Multiple-quantum-well-based photonic crystals with simple and compound elementary supercells

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Exciton polaritons in one-dimensional photonic crystals based on multiple quantum well structures are investigated. The effects due to interplay between resonant interaction of light with quantum well excitons, and light scattering from well-barrier interface, are elucidated. Polariton dispersion equations and reflection spectra in structures with two wells in an elementary supercell of the periodic structure are studied. Several examples of different compound elementary supercells are considered. Special attention is paid to structures with the period or the distance between quantum wells satisfying the resonance Bragg condition. Such structures are characterized by a presence of a larger-than-usual polariton stop band. It is shown that in structures with a complex elementary supercell, the width of such a stop band can be significantly enhanced in comparison to that in simple structures.

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I. INTRODUCTION

The physics of structures with periodically modulated dielectric permeability allowing for Bragg diffraction of light (photonic crystals) is an exploding field that attracts both fundamental and technological interests (see Ref. 1, and references therein). Depending upon the type of modulation one can consider three-, two-, or one-dimensional photonic crystals. In its simplest realization, a photonic crystal (PC) consists of two materials, A and B, with different indices of refraction, which are assumed to be constant in the frequency region of interest. One-dimensional photonic crystals of this kind are simply periodic multilayer structures, which were intensively studied in the past, but still attract significant attention. An assumption of frequency independent dielectric constant in such structures implies absence of internal excitations of the medium in a given frequency region; therefore, such structures are sometimes called passive photonic crystals. If, however, one of the materials constituting a PC has dipole active internal excitations in the PC’s operational frequency region, the assumption of constant indices of refraction breaks down, and one has to take into account frequency dispersion of the dielectric permeability. Such structures, which can be called optically active or resonant PC, were earlier considered in Refs. 6–8, and has recently been enjoying growing interest.

A special class of resonant PCs arises when one considers periodical structures with semiconductor quantum dots, quantum wires or quantum wells. External excitations in these materials are excitons affected by quantum confinement in zero, one, or two dimensions respectively. Multiple quantum wells (MQW), which form one-dimensional periodic structures, are of most interest from a practical point of view. This is because existing growing technologies allow for creating MQW structures of a very high quality with values of parameters that can be varied within a wide range. The main difference between multiple quantum wells and a passive one-dimensional PC lies in the role played by radiative coupling between excitons in different quantum wells. This coupling is particularly important when the period of the structure is comparable with the wavelength of light at the exciton frequency. In this case, radiation induces a strong coherent interaction between excitons of different wells, which leads to a significant modification of both dispersion of electromagnetic waves propagating in such a structure and radiative dynamics of the quantum well excitons. Particularly drastic changes occur in so-called Bragg MQW structures, in which oscillator strength of all but one mode vanishes, and the strength of coupling of the remaining mode with radiation becomes proportional to the number of wells in the structure.

In the limit of infinitely long periodic structures, the radiative coupling gives rise to a photonic band structure with the largest photonic stop-band in the vicinity of the exciton frequency. Since in this frequency region light most strongly interacts with excitons forming polaritons, we shall call this region a polariton stop-band. The formation of this polariton band-gap is not related to the scattering of light due to the spatial modulation of the refractive index; it exists even in the absence of a dielectric contrast between different layers of the structure. For this reason, the systems of this kind should be classified as a semiconductor analog of optical lattices, which are usually understood as periodic arrangements of atoms in vacuum or a homogeneous dielectric.

Thus, we can distinguish between two essentially different mechanisms of formation of band structure: periodically modulated coupling between light and internal excitations of a medium in optical lattices, and light scattering from spatial
inhomogeneities of dielectric constant in PCs. In real MQW structures, however, radiative coupling coexists with the dielectric mismatch between wells and barriers. Therefore, propagation of light in MQWs is controlled by an interplay between radiative coupling (optical lattice mechanism) and scattering from well-barrier interfaces (photonic crystal mechanism). While the contrast in the indices of refraction of wells and barriers was taken into account in some earlier calculations of the reflection coefficients of MQW structures and in the analysis of the modification of the exciton oscillator strength due to presence of cladding layers, the general picture of the polariton spectrum in such structures has not yet been elucidated. One of the objectives of this paper is to give a complete theory of polariton dispersion and optical spectra of optically active one-dimensional PC structures based on multiple quantum wells, in which radiative coupling and interface scattering play equally important roles.

Another important extension of the theory of resonant PCs, which we introduce in this paper, involves consideration of periodic structures with more than one well in an elementary supercell. While previous studies were mostly concerned with structures having a simple basis consisting of a single sphere, cylinder, or a quantum well, extending consideration to more complicated structures would give more flexibility in designing structures with desirable optical characteristics. It was shown, for instance, that by including one or several “defects” in an MQW structure (a well with different characteristics, increased distance between adjacent wells, etc.), one can significantly modify optical properties of the structures allowing for engineering spectra with predefined properties. Introducing structures with a complex basis further extends capabilities to design the optical properties of materials. From experimental and technological points of view, growing periodic MQW structures with several wells in a supercell does not involve significant difficulties, and actually such structures have already been studied experimentally in Refs. 28 and 29, where reflection of light from structures with alternating quantum wells of two kinds has been considered. In the present paper, we derive dispersion equations for exciton polaritons in one-dimensional MQW based photonic crystals with a complex basis consisting of several quantum wells, and analyze the reflection spectrum of such structures.

II. EXCITON POLARITONS IN MQW PHOTONIC CRYSTALS WITH A SIMPLE SUPERCELL: ROLE OF THE REFRACTIVE INDEX CONTRAST

As it has been explained in the Introduction, an accurate description of optical properties of MQW in the region of an exciton resonance requires taking into account both mechanisms of interaction between light and a MQW: radiative coupling to excitons and interface scattering due to mismatch between dielectric properties of well and barrier layers. The general effect of this mismatch on the exciton polaritons in long-period quantum well structures has been previously considered in Ref. 22. In particular, an expression for the transfer matrix \( \hat{T} \) was derived for a layer of the width \( d \) with a quantum well in its middle. A dispersion equation relating the Bloch wave number \( K \) and the light frequency \( \omega \) can be written in terms of the elements of this transfer matrix as

\[
\cos Kd = \frac{1}{2} (T_{11} + T_{22}),
\]

where \( T \) is the \( \omega \)-dependent transfer matrix through the period \( d \). Using results of Ref. 22 and assuming that the well and barrier layers have widths \( a \) and \( b \) and are characterized by indices of refraction \( n_a \) and \( n_b \), respectively, this equation can be presented in the following convenient analytical form:

\[
\cos Kd = G(\omega,a,b) = \frac{D_1 + D_2 S(\omega)}{1 - \frac{r_{ba}^2}{\cos^2 Kd}},
\]

where

\[
D_1 = \cos \phi_a - r_{ba}^2 \cos \phi_0 = (1 - r_{ba}^2) \left[ \cos \phi_a \cos \phi_0 - \frac{1}{2} \left( \frac{n_a}{n_b} + \frac{n_b}{n_a} \right) \sin \phi_a \sin \phi_0 \right],
\]

\[
D_2 = \sin \phi_a + r_{ba}^2 \sin \phi_0 - 2r_{ba} \sin \phi_0,
\]

\[
\phi_a = k_a a, \quad \phi_0 = k_0 b, \quad k_{a,b} = (\omega/c) n_{a,b}, \quad r_{ba} = (n_b - n_a)/(n_b + n_a),
\]

and the single-pole function \( S(\omega) \) is defined as

\[
S(\omega) = \frac{\Gamma_0}{\omega - \omega_0 + i\Gamma}.
\]

Hereafter \( \Gamma_0 \) and \( \Gamma \) denote exciton radiative and nonradiative decay rates, respectively. In the limit \( n_a \to n_b \) one has \( r_{ba} \to 0, \phi_a \to kd \) and \( G(\omega,a,b) \to G(\omega,d) \), where the function \( G(\omega,d) \) determines the polariton dispersion equation in the absence of the mismatch

\[
\cos Kd = G(\omega,d), \quad G(\omega,d) = \cos kd + S(\omega) \sin kd.
\]

On the other hand, in the absence of the exciton contribution, Eq. (2) transforms into the standard dispersion equation,

\[
\cos Kd = \frac{D_1(\omega)}{1 - r_{ba}^2},
\]

for the normal light waves in an optical superlattice. Equations (2) can be rewritten in two equivalent forms:

\[
\cos^2 Kd = \frac{D_1 D_4}{1 - r_{ba}^2} \quad \text{or} \quad \sin^2 Kd = \frac{D_5 D_6}{1 - r_{ba}^2}
\]

with factorized right-hand sides, where

\[
D_1 = \cos(\phi_a/2) - r_{ba} \cos(\phi_a/2), \quad D_4 = \sin(\phi_a/2) - r_{ba} \sin(\phi_a/2),
\]

\[
D_4 = \cos(\phi_a/2) + r_{ba} \cos(\phi_a/2) + S(\omega) \left[ \sin(\phi_a/2) - r_{ba} \sin(\phi_a/2) \right],
\]

\[
D_6 = \sin(\phi_a/2) + r_{ba} \sin(\phi_a/2) - S(\omega) \left[ \cos(\phi_a/2) - r_{ba} \cos(\phi_a/2) \right].
\]

These forms are particularly convenient for analyzing polar-
iton dispersion in quantum well structures, when exciton resonance frequency $\omega_0$ is close to a characteristic frequency $\bar{\omega}$ defined by

$$\bar{\omega}(n_b a + n_a)/c = \pi. \quad (9)$$

Naive consideration could lead to an expectation that this is the frequency at which the Bragg resonance in structures with the refraction index contrast would take place. Reality, however, is more complicated. Let us introduce the parameter $\xi = k_r \omega / a$ which can be rewritten as $(\bar{\omega}/c) n,a = \pi n d / (n_a + n_b b)$, see the definition (9). Assuming the parameter $\xi$ to be small, we can use in our analysis the following approximations:

$$\cos \frac{\phi_s}{2} = -\frac{\pi \omega - \bar{\omega}}{2 \bar{\omega}}, \quad \cos \frac{\phi_d}{2} = -\frac{\pi \omega - \bar{\omega} + \xi}{2 \bar{\omega}} + \xi,$$

$$\sin \frac{\phi_d}{2} \approx 1.$$

Solutions to the equations $D_1(\omega) = 0$ and $D_2(\omega) = 0$ give three exciton-polariton frequencies at the Brillouin zone edge $K = \pi/d$. Neglecting the nonradiative damping rate $\Gamma$ in (4), they can be written as

$$\omega_{1,2} = \omega_0 + \frac{1}{2} \left( \delta - \Omega' \right) \pm \frac{1}{2} \sqrt{\left( \delta - \Omega' \right)^2 + 4 n_a \Delta^2}, \quad (10)$$

$$\omega_3 = \bar{\omega} + \frac{n_b}{n_a} \Omega',$$

where

$$\delta = \bar{\omega} - \omega_0, \quad \Omega' = \frac{\xi (n_a - n_b) - \bar{\omega}}{m_{b1}} \text{ and } \Delta = \sqrt{\frac{2}{\pi \bar{\omega}}} \Gamma_0.$$  

In the absence of the dielectric-constant mismatch, Eq. (10) reduces to Eq. 12 in Ref. 16. The frequency at $K=0$ is found from the equation $D_3(\omega) = 0$ and given by

$$d_{14}(n_a, n_b) = d_{13}(n_b) + (n_a - n_b) \left[ \frac{\sin(\omega_0 n_b a/c)}{n_a + n_b + (n_a - n_b) \cos(\omega_0 n_b a/c)} - \frac{a}{n_b} \right], \quad (12)$$

where

$$d_{13}(n_b) = (\pi c/\omega_0 n_b) \quad (13)$$

defines a Bragg structure in the absence of the contrast. It can be shown that the period $d_{13}$ defined by Eq. (12) in fact satisfies the condition $D_1(\omega_0)/(1-r_{10}^\omega) = -1$ or $D_2(\omega_0) = 0$ similar to that given by Eq. 23 in Ref. 22. The physical meaning of this condition becomes clear if one realizes that in this case the exciton frequency $\omega_0$ coincides with the lower frequency boundary $\omega_{PC}$ of the respective band gap in a passive (i.e., without excitons) PC characterized by the same indices of refraction. Then the condition $\omega_0 = \omega_{PC}$ can be recast in the form

$$K_{PC}(\omega_0) d_{13} = \pi, \quad (14)$$

where $K_{PC}$ is the wave number of electromagnetic waves propagating in the respective PC. Equation (14) clearly demonstrates that the Bragg condition in MQW photonic crystals has essentially the same form as the one in optical lattices: wavelength of electromagnetic waves in a medium without...
excitons taken at the exciton frequency must be equal to the doubled period of the structure. The only difference is that in optical lattices, the wavelength is determined by a standard linear form for electromagnetic dispersion law, while in MQW PCs this dispersion law is determined by a dispersive equation, Eq. (6), for passive photonic crystals.

In the case of small contrast, the exact condition, Eq. (14) can be presented in a simple form \( \omega_0 = \omega_c - \Delta_r \), which is, of course, equivalent to Eq. (12). Here \( \omega_c = \pi c / [2(n_b + n_d)] \) is the center of the band gap in the passive PC and \( \Delta_r = 2 \omega_c f_{wa} \sin(\omega_c n_d / c) / \pi \) is the half-width of this gap. Analysis shows that taking into account radiative coupling between excitons does not change the position of the center of the band gap, which remains at frequency \( \omega_c \), but it modifies the half-width of the stop band. In the presence of both radiative coupling and the refractive index contrast, the half-width is given by the following expression:

\[
\Delta_r \approx \sqrt{\Delta_r^2 + \Delta_{OL}^2},
\]

where \( \Delta_{OL} \) is the half-width of the forbidden gap in structure without the contrast and is given by well-known expression\(^{12}\)

\[
\Delta_{OL} = \sqrt{2 \omega_0 L_0}. \tag{16}
\]

A single-gap miniband structure is also realized at \( \bar{\omega} \), satisfying the equation \( \omega_1 = \omega_2 \). It is a case of the accidental degeneracy of the two exciton-polariton states at the point \( K = \pi d / L \). Therefore, the disappearance of one forbidden gap can be considered an effect of crossing the states \( \omega_1 \) and \( \omega_2 \). Since these states have different symmetries (one is symmetric and another is antisymmetric with respect to the reflection in the interface plane), the states do not couple, and an expected anticrossing effect does not occur.

III. DISPERSION EQUATION FOR EXCITON POLARITONS IN MQW WITH COMPLEX ELEMENTARY SUPERCELL

In this section we analyze the dispersion properties of polaritons in MQW optical lattices with several wells in an elementary supercell. Thus, we neglect here the contrast in the indices of refraction of wells and barriers, which was studied in the previous section in the case of structures with a simple basis.

Let us enumerate the quantum wells in the periodic structure by the pair of indices \( m \) and \( j \), where \( m = \ldots , -2, -1, 0, 1, 2, \ldots \) numerates elementary supercells, and \( j = 1, 2, \ldots , n \) is the well’s number inside the supercell. As the elementary supercell, we choose a region between two planes shown by vertical dashed lines in Fig. 2. One of the planes lies in the middle between the centers of the last well in the supercell \( m-1 \) and the first well in the supercell \( m \), and the second plane is in the middle between the centers of the last well in the supercell \( m \) and the first well in the supercell \( m+1 \). The transfer matrix, \( \hat{T} \), for a supercell can be written as the product

\[
\hat{T}_j = \hat{T}_0(\bar{d}_j) + i \hat{S}_j(\omega) \hat{T}^*(\bar{d}_Rj, \bar{d}_Lj), \tag{20}
\]

where

\[
\hat{T}_j = \hat{T}_0(\bar{d}_j) + i \hat{S}_j(\omega) \hat{T}^*(\bar{d}_Rj, \bar{d}_Lj),
\]

\[
\hat{\mathcal{T}} = \prod_{j=1}^{n} \hat{T}_j,
\]

\[
\hat{T}_j = \frac{1}{t_j} \left( \begin{array}{cc} \hat{T}_j - R_{Lj} \hat{T}_j R_{Rj} & R_{Rj} \\ - R_{Lj} & 1 \end{array} \right),
\]

\[
t_j = e^{i \bar{d}_j} (1 + Z_j), \quad R_{Lj} = e^{i \bar{d}_Lj} Z_j, \quad R_{Rj} = e^{i \bar{d}_Rj} Z_j,
\]

\[
Z_j = \frac{i \Gamma_{0j}}{\omega_{0j} - \omega - i (\Gamma_{0j} + \Gamma_j)}.
\]

Here \( k = (\omega / c) n_p, n_b = e \epsilon_p, \Gamma_{0j} \) and \( \Gamma_j \) are the exciton radiative and nonradiative decay rates in the well of the sort \( j \) and \( d_{Lj} \) and \( d_{Rj} \) are the distances between the center of the \( j \)-th well and the center of the well situated to the left or to the right from the \( j \)-th well, respectively, \( \bar{d}_j = (d_{Lj} + d_{Rj}) / 2 \). Let us note that \( t_j^2 - R_{Lj} R_{Rj} = e^{2i \bar{d}_j(1 + 2Z_j)} \) and the matrix (18) can be presented in the form

\[
\hat{\mathcal{T}} = \hat{T}_0(\bar{d}_j) + i \hat{S}_j(\omega) \hat{T}^*(\bar{d}_Rj, \bar{d}_Lj),
\]
\[
\hat{T}_j(d_j) = \begin{pmatrix}
e^{i k d_j} & 0 \\
0 & e^{-i k d_j}\end{pmatrix},
\]
\[
\hat{T}'(d_{Rj},d_{Lj}) = \begin{pmatrix}
e^{-i k d_j} - e^{i (k d_j - k d_j)/2} \\
e^{i (k d_j - k d_j)/2} & e^{-i k d_j}\end{pmatrix},
\]
and
\[
S_j(\omega) = \frac{\Gamma_{0j}}{\omega - \omega_{0j} + i \Gamma_j}.
\]
Therefore each component of the transfer matrix \(\hat{T}_j(\omega)\) as a function of complex variable \(\omega = \omega' + i \omega''\) has the same pole of the first order at the frequency \(\omega_{0j} - i \Gamma_j\) where the transmission \(t_j\) is zero. Hence the sum \(T_{11} + T_{22}\) has poles of the first order at all frequencies \(\omega_{0j} - i \Gamma_j\) \((j = 1, \ldots, n)\) and this sum is real as soon as \(\Gamma_j = 0\) and the frequency \(\omega\) is real. This property allows one to represent rhs of Eq. (1) in the form
\[
\frac{1}{2}(T_{11} + T_{22}) = \cos kd + \sum_{j=1}^{n} C^{(m)}_j S_j(\omega),
\]
where the coefficients \(C^{(m)}_j\) are real. It is worthwhile to stress that the functions \(S_j(\omega)\) do not contain the radiative decay rates \(\Gamma_{0j}\) in their denominators, in contrast to \(Z_j(\omega)\). The reason is that, first, \(\Gamma_{0j}\) describes the strength of the photon-exciton interaction that leads to the formation of exciton polaritons and, secondly, in an infinite periodic structure and in the absence of the nonradiative decay, this interaction do not result in the absorption of the polaritons.

In a structure with one quantum well in the elementary supercell this dispersion law is reduced to Eq. (5), \(^{12}\) where the period \(d\) is merely the distance between the nearest quantum wells.

Here we present the dispersion equation for the normal light waves in a periodic structure with alternating quantum wells of two kinds (Fig. 2). After the substitution of Eqs. (18) and (19) to Eq. (22), the dispersion law can be reduced to a rather simple form:
\[
\cos^2(Kd/2) = G_1(\omega,d/2)G_2(\omega,d/2) - S_1(\omega)S_2(\omega)\sin^2(k \delta 2),
\]
where the period of the structure \(d\) is equal to the sum \(d_1 + d_2\), \(d_{12}\) are the distances between the nearest-neighbor wells (Fig. 2), \(\delta = d_2 - d_1\), and
\[
G_j(\omega,l) = \cos kl + S_j(\omega)\sin kl.
\]
In two particular cases, the dispersion equation (23) turns to Eq. (5). Indeed, if there are no excitonic states in the wells with even numbers, (i.e., \(\Gamma_{02} = 0\)), then Eq. (23) becomes
\[
\cos^2(Kd/2) = \cos(kd/2)G_1(\omega,d/2) \text{ or } \cos Kd = G_1(\omega,d)
\]
and, therefore, coincides with Eq. (5). Another limiting case is a structure with the identical wells 1 and 2 and \(d_{12} = d/2\). It is nothing more than a multiple quantum well-structure with the period \(d/2\) and one well in the elementary supercell. As a result, Eq. (23) reduces to Eq. (5), where the period \(d\) must be replaced by \(d/2\).

As has been shown in Ref. 13, a resonant Bragg structure with the period \(d_{Br}\) satisfying the condition given in Eq. (13) has a forbidden gap in the interval between the frequencies \(\omega_0 - \Delta\) and \(\omega_0 + \Delta\), where \(\Delta\) is given by Eq. (16) (in this section we drop subindex \(OL\)). In structures with the period \(d = N_{Br}\) exceeding that of a conventional resonant Bragg structure by the integer factor \(N\), the width of the forbidden gap 2\(\Delta\) decreases by a factor of \(\sqrt{N}\). This can be shown by expanding \(G(\omega,d)\) in Eq. (5) in powers of \(\omega - \omega_0\). In addition, it follows from Eq. (23) that, in structures with two identical wells in the elementary supercell and the interwell distances \(d_{12} = N_{Br}\), the width of the forbidden gap is given by \(2\sqrt{2/(N_1 + N_2)\Delta}\).

We provide the detailed analysis of Eq. (23) for a few specific structures. First of all, we consider the structures with the elementary supercells containing two identical quantum wells with arbitrary distances \(d_{12}\). In this case, the dispersion equation (23) can be rewritten in the form with a factorized right-hand side, namely,
\[
\cos^2(Kd/2) = D_kernel,
\]
where
\[
D_kernel = \cos(kd/2) + S(\omega)[\sin(kd/2) \pm \sin(k \delta 2)].
\]
There are several resonant structures satisfying particular conditions imposed on their geometrical characteristics. Let the period of the structure satisfy the Bragg condition, \(d = d_{Br}\). While analyzing the dispersion of exciton polaritons, we neglect the nonradiative exciton decay and set \(\Gamma = 0\). The sequence of allowed minibands and forbidden gaps is determined by the frequencies of exciton polaritons at the points \(K = 0\) and \(K = \pi/d\). The four frequencies at the edge of the Brillouin zone are solutions of the equation \(D_kernel = 0\), and they are given by
\[
\omega_+^1 = \omega_0 \pm \Delta \sqrt{1 + \sin(k \delta 2)}, \quad \omega_+^2 = \omega_0 \pm \Delta \sqrt{1 - \sin(k \delta 2)}.
\]
The two frequencies at the center of the Brillouin zone, \(K = 0\), are equal to \(\omega_-^1 = \omega_0 \pm k_0 \sec(k \delta 2)\). The interval between \(\omega_-^1\) and \(\omega_-^2\) is a narrow forbidden gap surrounded by a pair of allowed windows (or minibands):
\[
\omega_-^1 < \omega < \omega_-^2 \quad \text{and} \quad \omega_-^1 < \omega < \omega_-^2,
\]
which, in their turn, are sandwiched between the forbidden gaps
\[
\omega_-^1 < \omega < \omega_-^1 \quad \text{and} \quad \omega_-^2 < \omega < \omega_-^2.
\]
When decreasing the distance between the wells in the elementary supercell the allowed windows converge while the forbidden gaps increase and tend to \(\sqrt{2}\Delta\). This can be understood by taking into account that the limit \(d_{12} \to 0\) corresponds to the structure with one quantum well in the elementary supercell and the doubled exciton radiative decay rate, \(2\Gamma_0\). In the opposite case, where the wells are equally separated in the structure, the frequencies \(\omega_-^1, \omega_-^2\) (or \(\omega_-^1, \omega_-^2\)) coincide, and the lower and higher gaps disappear; only the central narrow gap survives. This result also follows from the
fact that when $d_1 = d_2$, the structure under consideration is the regular structure with a simple elementary supercell, but with the period two times smaller than the Bragg width $d_{Br}$. It corresponds to the so-called anti-Bragg case with the small gap $2\Gamma_0$.\textsuperscript{31}

The next resonance geometry concerns a structure with the period $d$ being twice as thick as the Bragg period and an arbitrary ratio $d_1/d_2$. In this case, there is one narrow gap embracing $\omega_0$ and two wide gaps on the opposite sides of $\omega_0$. To analyze the spectrum in the vicinity of this frequency, it is convenient to subtract unity from both parts of Eq. (23) and to transform this equation into $\sin^2(Kd/2) = D'_v D'_v$, with

$$D'_v = \sin(kd/2) - S(\omega)[\cos(kd/2) \pm \cos(kd/2)]$$ \hspace{1cm} (27)

The smallest gap is defined by the condition $|\omega - \omega_0| = \Gamma_0 |\sin(2\pi d_1/d)|$, while the wide gaps lie between the frequencies $\omega = \omega_0 \pm \Delta \sin(\pi d_1/d)$ and $\omega = \omega_0 \pm \Delta \cos(\pi d_1/d)$ as shown in Fig. 3. As $d_1 = 0$, $d_2$ or $d$, the wide gaps merge and form a single gap defined by $|\omega - \omega_0| \leq \Delta$. We note that here, in accordance with the discussion in the paragraph after Eq. (16), the band gap is $\sqrt{2}$ times smaller than in the case $d = d_{Br}$, $d_1 = 0$.\hspace{1cm}

The next example is a structure with two wells in the elementary supercell with the same values of the exciton frequencies and the nonradiative decay rates, $\omega_{01} = \omega_{02} = \omega_0$ and $\Gamma_1 = \Gamma_2 = \Gamma$, while the relation between $\Gamma_01$ and $\Gamma_02$ is arbitrary. Let the distances between the wells coincide, $d_1 = d_2 = d/2$, and satisfy the Bragg condition $(\omega_0/c)n_1(d/2) = \pi$. In the frequency region $|\omega - \omega_0| \ll \omega_0$, the dispersion of the exciton polaritons consists of two branches

$$\omega - \omega_0 = \pm \sqrt{\frac{1}{\pi} (\Gamma_01 + \Gamma_02) \omega_0 + \frac{1}{4\pi} \left(\frac{2\pi}{d} - K\right)^2} - i\Gamma,$$ \hspace{1cm} (28)

the same as in a periodic system of identical quantum wells with the period $d/2$, the exciton resonance frequency $\omega_0$ and the radiative decay rate $(\Gamma_01 + \Gamma_02)/2$.\hspace{1cm}

Now we consider a structure with a close pair of quantum wells, $d_1 \ll d_2 = d$, which differ both in the radiation decay rates $\Gamma_01$ and the exciton frequencies $\omega_0$. In the limit $\delta \to d$ Eq. (23) takes the form

$$\cos Kd = \cos kd + \frac{\Gamma_01}{\omega - \omega_01 + i\Gamma_1} + \frac{\Gamma_02}{\omega - \omega_02 + i\Gamma_2} \sin kd.$$ \hspace{1cm} (29)

It is interesting to compare this result with the polariton dispersion law in a structure with a simple elementary supercell, but with two exciton frequencies taken into account. In general, the coupling of the electromagnetic field with the excitonic states leads to the radiative decay rates $\Gamma_01$ and $\Gamma_02$ as well as to a renormalization of the exciton frequencies. However, if one neglects this renormalization, which is valid if $ka \ll 1$, where $a$ is the width of the quantum well, then the exciton dispersion relation coincides with Eq. (29).

As the final example, let us consider the same two-well compound structure, the interwell spacing $d/2$ and different exciton frequencies $\omega_{01}$ and $\omega_{02}$. The dispersion equation of the excitonic polaritons in such a structure has the simple form

$$\cos^2(Kd/2) = G_1(\omega, d/2)G_2(\omega, d/2).$$ \hspace{1cm} (30)

One can see that the set of polariton frequencies at the edge $K = \pi/d$ consists of those in the two independent structures with one quantum well, either 1 or 2, in the supercell and the period $d/2$. Assuming that $\Gamma_01 = \Gamma_02 = \Gamma_0$ and the period $d$ satisfies the Bragg condition at the average frequency $\bar{\omega} = (\omega_{01} + \omega_{02})/2$, (i.e., $\bar{\omega}_{01}, \bar{\omega}_{02} = \pi$), we obtain a set of four frequencies at $K = \pi/d$,

$$\omega_{1(4)} = \bar{\omega} + \frac{\omega_{21}}{4} \pm \sqrt{\frac{\omega_{21}^2}{4} + \Delta^2},$$ \hspace{1cm} (31)

where $\omega_{21} = \omega_{02} - \omega_{01}$ and $\Delta$ is defined according to Eq. (16). A special case, when two band gaps coalesce to form a single wide band gap, is realized when the frequency spacing $\omega_{21}$ equals $\sqrt{2}\Delta$. Under this condition, the width of the forbidden gap is $2\sqrt{2}\Delta$.

Using the general Eqs. (1), (18), and (19), one can prove that, for periodical structures containing $n = 2, 3, 4, \ldots$ quantum wells in the elementary supercell with equal distances $d/n$ between them, the dispersion equations take the form

$$\cos Kd = 2G_1(2)^2G_2(2)^2 - 1 \quad (n = 2),$$ \hspace{1cm} (32)
\[
\cos Kd = 4G_1^{(3)}G_2^{(3)}G_3^{(3)} - (G_1^{(3)} + G_2^{(3)} + G_3^{(3)}) \quad (n = 3),
\]

(32)

\[
\cos Kd = 8G_1^{(4)}G_2^{(4)}G_3^{(4)}G_4^{(4)} - 2(G_1^{(4)}G_2^{(4)} + G_2^{(4)}G_3^{(4)} + G_3^{(4)}G_4^{(4)}) + G_4^{(4)}G_1^{(4)} + 1 \quad (n = 4),
\]

where

\[
G_j^{(n)}(\omega) = G_j(\omega, d/n) = \cos(kd/n) + \sin(kd/n)S_j(\omega).
\]

(33)

Formally, the structure of the right-hand sides of these equations can be obtained by expanding \( \cos kd \) with respect to powers of \( \cos(kd/n) \).

\[
\cos kd = \sum l M_l^{(n)} \cos(kd/n) = 2^{n-1} \cos^n(kd/n)
\]

\[
- \frac{n}{1!} 2^{n-3} \cos^{n-2}(kd/n) + \frac{n(n-3)}{2!} 2^{n-5} \cos^{n-4}(kd/n)
\]

\[
- \frac{n(n-4)(n-5)}{3!} 2^{n-7} \cos^{n-6}(kd/n) + \cdots
\]

and replacing \( \cos(kd/n) \) by symmetrized products of \( l \) functions \( G_j^{(n)}(\omega) \), so that \( \cos^{n-2}(kd/n) \) turns to

\[
\cos^{n-2}(kd/n) \rightarrow \frac{1}{n} \left[ U_n(1;n - 2) + U_n(2;n - 1) + U_n(3;n) + \cdots + U_n(n;2n - 3) \right],
\]

(34)

where

\[
U_n(l;n - l') = \prod_{j=l}^{n-l'} G_j^{(n)}, \quad U_n(l;n + l') = U_n(1;n) \frac{U_n(1;l')}{U_n(1;l - 1)}.
\]

(35)

The coefficient \( M_{l=0}^{(n)} \) independent of \( \cos(kd/n) \) remains unchanged. Let us note that Eq. (32), for \( n=2 \) coincides with Eq. (30) since \( \cos^2(Kd/2) = (1 + \cos Kd)/2 \).

Taking into account PC effects (refraction index contrast) in systems with complex elementary supercells makes a consideration of the polariton spectrum much more complicated. Therefore, we will restrict ourselves by presenting here a general form of the polariton dispersion equation for a two-well structure, which in the optic lattice case is described by Eq. (30). Taking the contrast of the indices of refraction into account, we have to introduce separately well and barrier thicknesses, \( a_j, b_j \), which, however, in this structure are independent of \( j \), i.e., \( a_1 = a_2 = a, b_1 = b_2 = b \) so that the period of the structure equals \( 2(a + b) \). The dispersion equation for exciton polaritons in this case can be written as

\[
\cos^2(Kd/2) = G_1(\omega, d/2)G_2(\omega, a, b)
\]

\[
+ \frac{F_1 + F_2S_1(\omega) + F_3S_2(\omega) + F_4S_3(\omega)S_2(\omega)}{1 - r_{ba}^2},
\]

(36)

where

\[
F_1 = 1 - \cos(k_\omega a) - r_{ba}^2[1 - \cos(k_\omega a)],
\]

\[
F_2 = -[\sin(k_\omega a) + 2r_{ba} \sin(k_\omega a) + r_{ba}^2 \sin(k_\omega a)],
\]

\[
F_3 = \sin(k_\omega a) + 2r_{ba} \sin(k_\omega a) - r_{ba}^2 \sin(k_\omega a),
\]

\[
F_4 = 1 - \cos(k_\omega a) + 2r_{ba}[\cos(k_\omega a) - \cos(k_\omega a)]
\]

\[
+ r_{ba}^2[1 - \cos(k_\omega a)],
\]

\[k_\omega = k_\varphi \pm k_\parallel \] One can check that, at \( n_a \rightarrow 0 \), this equation transforms into Eq. (30). The numerical solution of this equation will give form of polariton spectrum, including positions and widths of polariton stop bands. A more detailed analysis of this equation will be presented elsewhere.

**IV. REFLECTION SPECTRA**

The reflection spectrum of a structure containing 10 pairs of identical quantum wells is shown in Fig. 4. The calculation has been performed using the following parameters: \( d = 2d_{Br}, d_1/d = 0.1, \Gamma_p = \Gamma = 7 \times 10^{-5} \omega_0 \). We have taken into account that the transfer matrix for any symmetrical inhomogeneous layer can be written in terms of its reflection (\( \mathcal{R} \)) and transmission (\( \mathcal{T} \)) coefficients as

\[
\mathcal{T} = \frac{1}{\mathcal{R}} \begin{pmatrix} \mathcal{T}^2 - \mathcal{R}^2 & \mathcal{R} \\ -\mathcal{R} & 1 \end{pmatrix}.
\]

(37)

For a layer of the width \( d \) with two identical quantum wells inserted symmetrically inside the layer, the coefficients \( \mathcal{R} \) and \( \mathcal{T} \) have the form

\[
\mathcal{R}_2 = i e^{ikd} \left( \frac{1 - \cos \phi}{\Omega + i(1 - \eta)} - \frac{1 + \cos \phi}{\Omega + i(1 + \eta)} \right),
\]

(38)
\[ T_2 = e^{i k d} \left[ 1 - i \left( \frac{1 - \cos \phi}{\Omega + i(1 - \eta)} + \frac{1 + \cos \phi}{\Omega + i(1 + \eta)} \right) \right], \]

where \( \Omega = (\omega - \omega_0 + i \Gamma_0)/\Gamma_0, \phi = k d_1, d_1 \) is the interwell distance and \( \eta = e^{i \phi} \).

Figure 4 shows the reflection spectrum from \( N \) such pairs with the period satisfying the double Bragg condition \( k(\omega_0) d = 2 \pi \). The transfer matrix \( \hat{T}^{(N)} \) of such a system has the same form (37), with \( R \) and \( T \) replaced by the reflection (\( R_N \)) and transmission (\( T_N \)) coefficients of the whole system. This transfer matrix is obtained from the transfer matrix through a single supercell by raising the latter to the \( N \)th power. If one neglects a small frequency variation of the wave vector \( k(\omega) = n_1 \omega/c \) and replaces \( k(\omega) d \) with \( 2 \pi \) then one can see that the coefficients \( R_N = |R_N|^2 \) and \( T_N = |T_N|^2 \) as functions of \( \omega \) and \( d_1/d \) possess some important symmetry properties. First, the substitution \( d_1/d \to (1/2) + (d_1/d) \) leads to

\[ \sin \phi \to -\sin \phi, \cos \phi \to -\cos \phi, \eta \to -\eta, \]

and, therefore,

\[ R_2 \to -R_2, T_2 \to T_2, \hat{T}^{(N)} \to \hat{T}^{(N)}\Tilde{,} \]

\[ R_N(\omega - \omega_0; d_1/d) = \frac{T_N^{(N)}}{T_{12}^{(N)}}, \]

because \( |T_N^{(N)}| = |T_{12}^{(N)}| \). Similarly, the change

\[ d_1/d \to \frac{1}{2} + \frac{d_1}{d}, \]

leads to

\[ \omega - \omega_0 \to (\omega - \omega_0), \sin \phi \to -\sin \phi, \cos \phi \to -\cos \phi, \]

\[ R_2 \to -R_2, T_2 \to T_2, \hat{T}^{(N)} \to \hat{T}^{(N)\Tilde{}} \]

and, as a result,

\[ R_N(\omega - \omega_0; d_1/d) = R_N(\omega_0 - \omega; 1/2 + d_1/d) = R_N(\omega_0 - \omega; 1 - d_1/d). \]

Let us notice that infinite periodic structures with the interwell distance in the elementary supercell equal to \( d_1 \) and \( -d_1 \) are identical. Meanwhile, such structures with a finite number, \( N \), of quantum wells are not. Indeed, the first structure, with the distance \( d_1 \), can be denoted by 1212...12, where the numbers 1 and 2 enumerate the wells in the elementary cells. The second one with the interwell distance \( d - d_1 \) can be presented as 2121...21 (i.e., it contains \( N \)−1 pairs 12 with two additional wells 2 and 1 grown at the distance \( d_2 = d - d_1 \) from the leftmost well 1 and the rightmost well 2, respectively). For large enough values of \( N \), the effect of the last well on the reflection coefficient \( R_N \) can be neglected. On the contrary, the first well can change \( R_N \) significantly and, thus, values \( R(\omega - \omega_0; d_1/d) \) and \( R(\omega_0 - \omega_0; d_1/d) \) differ due to this front-well effect.

Two wide peaks in Fig. 4 are caused by two forbidden gaps in the spectrum of the infinite periodic structure (see Fig. 3). The values of \( R_N \) differ from 1 at these regions due to a finite exciton nonradiative decay. Approximately one spectral peak can be obtained from the other by reflection in the vertical line passing through the resonance frequency \( \omega_0 \). With increasing \( N \), this symmetry property improves. However, in the vicinity of \( \omega_0 \) the spectrum is essentially asymmetric. The asymmetry survives even in the limit \( N \to \infty \). This result follows from a comparison of the coefficients \( R_N(\omega - \omega_0; d_1/d) \) and \( R_N(\omega - \omega_0; 1 - d_1/d) \). Indeed, the semi-infinite structure 212... differs from the structure 2121... by the front well. As a result, \( R_N \) and \( R'_N \) can be related by

\[ R'_N = e^{i k d} \left[ r + \frac{\tau^2 R_N e^{i k d_2}}{1 - r R_N e^{i k d_2}} \right] \]

where \( r = Z i [\omega - \omega_0 - i(\Gamma_0 + \Gamma)] \) and \( \tau = 1 + r \) are the reflection and transmission coefficients for a single well, \( R_N = R_N/(1 - T_N e^{i k d_2}) \), and \( K \) is the wave vector of an exciton polariton at the frequency \( \omega \) in the infinite structure. One can see that the absolute values \( R_N \) and \( |R'_N| \) are different due to the second term in the right-hand side of Eq. (41), which is proportional to \( r \) and has the half-width of the order of \( \Gamma_0 + \Gamma \). Taking into account the symmetry relation (40), one can say that the values of the reflectivity \( R_N \) at the frequencies \( \omega = \omega_0 \pm \delta \omega \) can essentially differ in the region \( \delta \omega \sim \Gamma_0 + \Gamma \). The calculation illustrated in Fig. 4 confirms this conclusion.

If the nonradiative decay is neglected, \( \Gamma = 0 \), one has a total reflection in the region of the forbidden gaps. In this case, the coefficients \( R_N \) and \( R'_N \) can be represented as \( \exp(i \phi) \) and \( \exp(i \Phi') \) respectively, where the phases \( \Phi, \Phi' \) are complicated functions of the frequency. It follows from Eq. (41) that they are related by

\[ \Phi' = \Phi + kd + 2 \arctan \frac{\Gamma_0[1 + \cos(\Phi + kd_2)]}{\omega_0 - \omega + i \Gamma_0 \sin(\Phi + kd_2)}. \]

In the frequency region between the wide peaks, the reflectivity \( R(\omega) \) contains a set of narrow maxima and minima. As \( N \to \infty \), the set turns into a pair of narrow maximum and minimum located symmetrically with respect to \( \omega_0 \).

The reflection coefficient of a pair of wells with the distance \( d_1 \) between them, satisfying the Bragg condition and with the same values of \( \omega_0 \) and \( \Gamma \) but with different radiative decay rates \( \Gamma_0 \neq \Gamma_0 \), coincides with the reflection coefficient of a single well with the radiative decay rate equal to \( \Gamma_0 + \Gamma_0 \). Therefore the reflectivity of a structure with \( N \) such pairs and the period \( d = 2 d_1 \) is the same as that of a resonant Bragg structure with \( 2 N \) identical wells, characterized by the exciton radiative decay rate \( (\Gamma_{01} + \Gamma_{02})/2 \).
In this paper, the theory of multiple quantum well photonic crystals has been developed in two directions. First, we gave a complete picture of a polariton spectrum in systems where radiative coupling of excitons and interface scattering of electromagnetic waves due to refraction index contrast between wells and barriers play equally important roles. We clarified the physical meaning of the Bragg condition in this case, and showed that it can be formulated in the form of a standard relation between wavelength of exciton radiation and the period of the structure. In this relation, however, the wavelength should be determined from a modified dispersion equation describing electromagnetic waves in a passive (i.e., without excitons) photonic crystals. In the approximation of small contrast, we found a simple expression for the width of the polariton stop band, which turned out to be equal to a “pythagorean” sum of band widths of respective optical lattice and passive photonic crystal.

Second, we developed a theory of exciton polaritons in compound one-dimensional photonic crystals. It has been shown that the dispersion equation has the form \( kd = F(\omega) \), where \( F(\omega) \) as a function of the complex frequency \( \omega \) has poles at the resonance frequencies \( \omega_{j} - \omega_{0} \), of the “mechanical” excitons in quantum wells \( j = 1, 2, \ldots \) constituting the elementary supercell. In important particular cases, \( F(\omega) \) can be represented in an analytical form, permitting one to investigate explicitly the dependence of the polariton spectrum and the structure of the forbidden minigaps upon the exciton parameters and the geometrical characteristics of the photonic crystal. This investigation allows one to draw a conclusion that the compound structures are promising from the application point of view, because at the same length of the period of the structure the forbidden gap and, therefore, the modification of the electromagnetic wave spectrum due to interaction with excitons can be essentially amplified.

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\[ \text{FIG. 5. The effect of the difference between the exciton frequencies } \omega_{01} \text{ and } \omega_{02} \text{ on the reflection spectrum of the structure with } 10 \text{ pairs of the quantum wells with equal both radiative and nonradiative decay rates } \Gamma_{02} = \Gamma_{1} = \Gamma_{2} = 7 \times 10^{-5} \omega_{01}. \text{ The quantum wells are equidistant and the period meets the Bragg condition at the frequency } \omega_{01}. \text{ The curves 1–5 have been obtained for } (\omega_{02} - \omega_{01})/\omega_{01} = 0, 0.002, 0.005, 0.01, \text{ and } 0.015 \text{ correspondingly.} \]

\[ \text{the wells be situated equidistantly, and the distance between them } d_{j} = d/2 \text{ meets the resonant Bragg condition for the frequency } \omega_{01}, \text{ i.e., } k(\omega_{01})d_{j} = \pi. \text{ When frequencies } \omega_{01} \text{ and } \omega_{02} \text{ coincide, the reflection coefficient of the structure consisting of } N \text{ pairs equals to the reflection coefficient of a Bragg structure with } 2N \text{ identical wells and has a Lorentz-type shape with half-width } 2N\Gamma_{0} + \Gamma. \text{ When } \omega_{02} = \omega_{01} \text{ and } |\omega_{02} - \omega_{01}| > \max\{\Gamma_{0}, \Gamma\} \text{ the reflection peak splits onto two narrower peaks at the frequencies } \omega_{\text{max,1}} = \omega_{01} \text{ and } \omega_{\text{max,2}} = \omega_{02}, \text{ with the half-widths close to } N\Gamma_{0} + \Gamma. \text{ Each peak is produced by the corresponding subsystem of quantum wells. With increasing the difference } \omega_{02} - \omega_{01}, \text{ the peak at } \omega_{01} \text{ becomes more symmetric while the second peak reveals a narrow dip near } \omega_{\text{max,2}}. \text{ Such a spectrum is reminiscent of spectra obtained in Refs. 24, 25, and 27 for systems with so-called } \Omega \text{-defects, in which one or several wells are replaced with wells characterized by a different exciton frequency. This resemblance can be understood by realizing that the system considered here is a structure, in which the } \Omega \text{-defects are introduced in place of every other well.} \]