Exciton–photon interaction in a quantum dot embedded in a photonic microcavity

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Abstract
We present a detailed analysis of exciton–photon interaction in a microcavity made out of a photonic crystal slab. Here we have analysed a disc-like quantum dot where an exciton is formed. Excitonic eigen functions in addition to their eigen energies are found through direct matrix diagonalization, while wavefunctions corresponding to unbound electron and hole are chosen as the basis set for this procedure. In order to evaluate these wavefunctions precisely, we have used the $6 \times 6$ Luttinger Hamiltonian in the case of hole while ignoring bands adjacent to the conduction band for electron states. After analysing excitonic states, a photonic crystal-based microcavity with a relatively high quality factor mode has been proposed and its lattice constant has been adjusted to obtain the prescribed resonant frequency. We use a finite-difference time-domain method in order to simulate our cavity with sufficient precision. Finally, we formulate the coupling constants for the exciton–photon interaction both where intra-band and inter-band transitions occur. By evaluating a sample coupling constant, it has been shown that the system can be in a strong-coupling regime and Rabi oscillations can occur.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
Cavity quantum electrodynamics (CQED) has been a central topic of intense research since the early 1990s, especially in optoelectronics and solid-state physics [1–7]. Recently, several experiments have been conducted in order to observe striking phenomena related to interactions occurring in such systems, and have addressed their possible applications in various regimes [8–14]. Generally speaking, in the weak coupling regime spontaneous emission can be enhanced or reduced compared with its vacuum level. However, in the strong-coupling regime the key signature is Rabi splitting, which is observed in the emission spectrum in the form of an anti-crossing between the quantum dot exciton and cavity-mode dispersion relations. In other words, Rabi oscillations occur in the decay dynamics, which take place before decoherence mechanisms.

Realization of single-photon sources as well as Q-bits, cryptography, quantum repeater, quantum computation and information are the main fields in which these phenomena seek application [11–17]. In most of these researches, photonic crystal (PhC)-based cavities and waveguides are exploited owing to their favourable properties. There are several reports dealing with the design of PhC-based cavities with specific properties for special applications in CQED. These criteria include a high quality factor and a low mode volume, which are met through geometrical manipulations [18–22].

An exciton–photon interaction in a PhC waveguide and a semiconductor quantum well (QW) as a two-dimensional system have been investigated theoretically in the literature [23, 24]. Also the possibility of Rabi splitting predicted by theoretical models in the strong-coupling regime has been verified experimentally for semiconductor quantum dots in cavities [25–29]. A recent review paper by Reithmaier summarizes the progress made in the area of strongly coupled nano-cavities, to which the reader is referred for more details [28].

We had made an initial attempt to investigate the quantum optical behaviour of exciton–photon interaction in photonic crystals, where the interaction with Bloch modes were analysed [30]. The authors had shown the formation of dressed states and Rabi oscillations, in the strong-coupling regime. The present study, however, extends the latter research without making any approximations, taking the exact nature of excitonic wavefunctions as well as photonic confined modes into account. In this paper, we investigate the exciton–photon
interaction in a disc-like quantum dot (QD) embedded in a 2D photonic crystal slab. The main motivation of this paper is to present a fundamental approach to design and understand the operation of such a cavity based on a basic theoretical method of the quantum optical and quantum mechanical phenomena involved. We show that it is possible to obtain an interaction within the strong-coupling regime, which allows a wide range of applications as mentioned above. We discuss the detailed design of the quantum dot as well as the photonic crystal cavity. Finally, the photon–exciton coupling rate has been computed and dressed (entangled) exciton–photon states are found.

In section 2, we investigate excitonic states through the diagonalization method and use unentangled electron and hole wavefunctions as the basis set. In section 3, a high quality factor PhC-based cavity has been designed, one of whose wavefunctions as the basis set. In the range of several to thousands of meV [31]. The exciton Bohr radius. The exciton’s binding energy may be equal. Excitons can be classified into Frenkel or Wannier types according to the average electron–hole distance called the critical point where the electron and hole group velocities are equal. Excitons can be formed by photon absorption at any point of an exciton, which is electrically neutral but can transport the electron–hole pair resides. In our case the material is GaAs and hence \( \epsilon_r = 13.2 \). The surface polarization of the QD has been ignored in (1) [32]. The eigenvectors corresponding to single particle Hamiltonian \( \hat{H}_e \) and that of \( \hat{H}_h \) form a complete basis set for their own subspace. Hence every vector belonging to the exciton space on which \( \hat{H}_X \) operates, can be spanned by the tensor product of these eigenvectors. Particularly, the \( \rho \)-th exciton Hamiltonian eigenvector \( |\psi^X_\rho\rangle \) could be expanded in this space as

\[
|\psi^X_\rho\rangle = \sum_{O,L} A^O_{\rho,L} |\psi^O_\rho\rangle \otimes |\psi^L_\rho\rangle. \tag{3}
\]

In the above expansion \( |\psi^O_\rho\rangle \) and \( |\psi^L_\rho\rangle \) stand for the \( O \)-th and \( L \)-th eigenvectors correspond to the electron and hole Hamiltonians, respectively. Note that in a QD structure, \( O \) and \( L \) are collective indices, each standing for three quantum numbers. Also \( A^O_{\rho,L} \) are the expansion coefficients. Equation (3) implies that an entangled electron–hole pair, i.e. an exciton, exists only if at least two expansion coefficients are nonzero. In view of the fact that our QD dimensions are big enough to encompass many atoms in all directions we are encouraged to assume an envelope function approximation (EFA) in order to obtain single particle wavefunctions.

In the case of electron states, since the conduction band is not degenerate in the non-relativistic regime and other bands are far enough, the Bloch part of the wavefunction can be chosen as an S-like orbital. So it is reasonable to ignore the adjacent bands, use only the conduction band and simply solve the Schrödinger equation for a single envelope function.

It is straightforward to obtain the following projection of electron states on the position bra owing to the simple QD structure

\[
|r_e\rangle|\psi^O_\rho\rangle = A e^{i\epsilon r_e J_n} \left( \frac{\beta_{\rho,n,r_e}}{R_0} \right) \sum_{\nu} Z^O_{\nu}(z_e) \chi^O(r_e). \tag{4}
\]

Here, \( J_n \) is the Bessel’s function of order \( n \), \( \beta_{\rho,n,r_e} \) is the \( \nu \)-th zero of \( J_n \) and \( R_0 \) is the radius of our disc-like QD. Also \( Z^O_{\nu} \) is the \( \nu \)-th envelope function along the QD’s height, i.e. the \( z \)-direction, which is sinusoidal inside the dot and exponentially decaying outside. So \( O \) stands for \( n, \nu \) and \( d \)-quantum numbers, collectively. Also, \( \chi^O \) stands for the S-like Bloch function and \( A \) is the normalization constant. The subscript \( e \) is here used for the three position coordinates of electron, \( \psi, \rho \) and \( z \) in the cylindrical coordinate. Also \( r_e \) stands for the aforementioned coordinate parameters collectively.

In contrast, the Bloch part corresponds to the hole wavefunction mainly composed of \( P_x \), \( P_y \) and \( P_z \)-like orbitals. The reason is that the valence band is not only twofold degenerate at the \( \Gamma \) point due to heavy hole (HH) and light hole (LH) bands, but also the spin–orbit split-off (SO) band may be close to these bands in some semiconductor band structure and has a significant contribution in the Bloch part of the hole wavefunction.

In order to obtain hole wavefunctions accurately, one needs to take the effect of these neighbouring bands into account. For the purpose of calculating envelope functions...
corresponding to each of these Bloch parts, the Luttinger Hamiltonian could be exploited. It is possible to use the Luttinger Hamiltonian in the cylindrical coordinate, because the radius of QD is an order of magnitude bigger than its thickness, we only employ it in the \( z \)-direction, i.e. along QD’s height [33]. In the \( xy \)-plane we still use the single band approximation which results in similar outcomes to that of electrons. Also, we take the effects of only three adjacent bands, i.e. HH, LH and SO, into account and hence deal with the \( 6 \times 6 \) Luttinger Hamiltonian. For more accuracy one can also take the conduction band into consideration and use the \( 8 \times 8 \) Luttinger Hamiltonian, but as long as the semi-conductor gap is large, the consequent improvement in modelling is negligible. This can readily be discerned from variational theory [34].

Irrespective of the method used to find the eigenvectors of the Luttinger Hamiltonian, we can write the hole wavefunction as

\[
| r_b \rangle \psi^h_L = A e^{i\varphi_S} J_m \left( \frac{\beta_{mc} \rho_h}{R_0} \right) \sum_k Z^h_{b,z}(z_h) \chi^h_k(r_h). \tag{5}
\]

Here, the summation runs over the number of considered bands multiplied by two due to the spin of electrons and holes. Here \( Z^h_{b,z}(z_h) \) is the \( h \)th component of the Luttinger Hamiltonian eigenvector corresponding to the \( h \)th bound envelope function along the QD’s height. Other parameters are defined similar to that of (4), except that the index \( e \) is replaced with \( h \), indicating the position of the hole instead of the electron. It is a common practice to diagonalize the \( 6 \times 6 \) Luttinger Hamiltonian matrix and achieve a \( 3 \times 3 \) block diagonal matrix through a unitary transformation [35–37]

\[
H^6_{\Gamma} = \begin{pmatrix} H^L_{\Gamma} & 0 \\ 0 & H^A_{\Gamma} \end{pmatrix}. \tag{6}
\]

In order to simplify the problem we also employ this procedure so that the reduced Hamiltonian reads

\[
H_{\Gamma}^c = \begin{pmatrix} P + O + V & R \mp iS \\ R \pm iS^\dagger & P - O \mp iC + V \end{pmatrix} \sqrt{\mathcal{T}R} \mp \frac{i}{2} \mathcal{T}S, \tag{7}
\]

in which \( \Delta_{so} \) is the spin–orbit splitting at the \( \Gamma \) point. Other parameters are given by

\[
P = \left( \frac{\hbar^2}{2m_0} \right) \gamma_1 \left( k_z^2 + k_x^2 + k_y^2 \right), \tag{8a}
\]

\[
Q = \left( \frac{\hbar^2}{2m_0} \right) \gamma_2 \left( k_x^2 + k_y^2 - 2k_z^2 \right), \tag{8b}
\]

\[
R = -\sqrt{3} \left( \frac{\hbar^2}{2m_0} \right) \gamma_0 k_z^2, \tag{8c}
\]

\[
S = 2\sqrt{3} \left( \frac{\hbar^2}{2m_0} \right) \kappa_1 \left( \sigma - \delta \right) k_z + k_z \pi, \tag{8d}
\]

\[
\Sigma = 2\sqrt{3} \left( \frac{\hbar^2}{2m_0} \right) k_z \left\{ \frac{1}{3} \left( \sigma - \delta \right) + \frac{2}{3} \pi \right\} k_z + k_z \left( \frac{2}{3} \left( \sigma - \delta \right) + \frac{1}{3} \pi \right), \tag{8e}
\]

\[
C = 2 \left( \frac{\hbar^2}{2m_0} \right) k_z \left[ \gamma_z, (\sigma - \delta - \pi) \right], \tag{8f}
\]

\[
\gamma_0 = \sqrt{\mathcal{P}^2 + \mu^2 - 2\mathcal{P} \mu \cos(\varphi)}, \tag{8g}
\]

\[
\mathcal{P} = \frac{\gamma_1 + \gamma_2}{2}, \quad \mu = \frac{\gamma_1 - \gamma_2}{2}, \tag{8h}
\]

\[
\sigma = \mathcal{P} - \frac{1}{2} \delta, \quad \pi = \mu + \frac{3}{2} \delta, \tag{8i}
\]

\[
\delta = \frac{1}{9} \left( 1 + \gamma_1 + \gamma_2 - 3\gamma_3 \right). \tag{8j}
\]

\[
\varphi = \arctan \left( \frac{k_x}{k_z} \right). \tag{8k}
\]

Also \( \left[ \right] \) stands for the commutation of two operators and \( \gamma_i \) are the Luttinger parameters. Besides, \( k_1 \) is the modulus of the in-plane wave vector, i.e. \( k_1 = \sqrt{k_x^2 + k_y^2} \), and \( m_0 \) is the electron rest mass. Table 1 enumerates these parameters for two materials constructing our QD.

We have also employed linear interpolation for ternary composition Ga\(_{0.25}\)Al\(_{0.75}\)As wherever applicable, and taken the influence of six strain components, i.e. \( \varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{xz}, \varepsilon_{yz}, \) and \( \varepsilon_{xy} \), into account by adding the Pikus–Bir deformation potentials to the main Hamiltonian. It can be accomplished by adding the following potential to their corresponding counterpart [38], given by:

\[
P_e = -a_e (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}), \tag{9a}
\]

\[
O_e = -\frac{b}{2} (\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz}), \tag{9b}
\]

\[
R_e = \frac{\sqrt{3}b}{2} (\varepsilon_{xx} - \varepsilon_{yy} - i\varepsilon_{xy}), \tag{9c}
\]

\[
S_e = -d (\varepsilon_{xx} - i\varepsilon_{yz}), \tag{9d}
\]

Here, \( a_e, b \) and \( d \) are the Pikus–Bir deformation potentials describing the hydrostatic, uniaxial and shear strain, respectively. Owing to our rather planar QD structure we may take \( \varepsilon_{yz} \approx \varepsilon_{zx} \), and ignore the effect of \( S_e \) or equivalently \( d \). The corresponding parameters for GaAs and AlAs are listed in table 2 [39].

### Table 1. Luttinger parameters for GaAs and AlAs.

| Parameter | \( \gamma_1 \) | \( \gamma_2 \) | \( \gamma_3 \) | \( \Delta_{so} \) (meV) |
|-----------|----------------|----------------|----------------|------------------------|
| GaAs      | 6.98           | 2.06           | 2.93           | 341                    |
| AlAs      | 3.76           | 0.82           | 1.42           | 280                    |

### Table 2. Pikus–Bir parameters for GaAs and AlAs.

|          | \( a_e \) | \( b \) |
|----------|----------|--------|
| GaAs     | -1.116 eV| -2.0 eV|
| AlAs     | -2.47 eV | -2.3 eV|


Since our QD can be considered as a layered structure in the $z$-direction, we used the transfer matrix method (TMM) in order to obtain the eigenstates of the Hamiltonian (7) \[40\]. Note that the upper and lower blocks in equation (6), are related through complex conjugate operator, i.e. $H^* = (H^T)^*$. Therefore, the eigenvectors of one, e.g. $H^*$, can be achieved upon determination that of another through complex conjugate transformation. Henceforth we will focus on the upper block eigenvalue problem, i.e. $H^*F = EF$. It is straightforward to decompose $H^*$ in three terms with respect to $k_z$

$$H^* = H_2k_z^2 + H_1k_z + H_0.$$ \(10\)

If we assume a constant potential profile in each layer, then all $k_z$ coefficients will be constant matrices. The eigenvalue problem results in a three-coupled second-order differential equation in terms of $k_z$. It is possible to reduce the differential equation order by introducing $\Phi = [F, F']^T$ at the cost of increasing the number of coupled equations to six. If so, the governing equation for $\Phi$ reads

\begin{equation}
\Phi' = \Lambda \Phi \tag{11a}
\end{equation}

\begin{equation}
\Lambda = \begin{pmatrix} O & I \\
H_2^{-1}(H_0 - E) & -iH_2^{-1}H_1 \end{pmatrix} \tag{11b}
\end{equation}

Note that $\Lambda$ is not diagonal and hence the above equation cannot be solved directly. It can be decomposed as

$\Lambda = PD^{-1}P^T$.

Here $D$ is a diagonal matrix composed of $\Lambda$ eigenvalues. Also $P$ is a square matrix composed of eigenvectors corresponding to $\Lambda$. Note that this decomposition is not unique. We choose $D$ so that its upper and lower half contains elements with positive and negative real parts, i.e. forward and backward propagating waves, respectively. By introducing another change of variable, i.e. $Q = P^{-1}\Phi$, equations (11a), (11b) recast in $Q' = DQ$ with the following solution:

$$Q = e^{DQ_0}.$$ \(12\)

It is evident that envelope wavefunction and probability current continuity boundary conditions across an interface should be imposed on $\Phi$, rather than $Q$. Assuming that Bloch parts across interfaces remain unchanged, it is straightforward to write

$$B_l\Phi(z_L) = B_R\Phi(z_R),$$ \(13\)

where the boundary condition matrix $B$ defined as

$$B = \begin{pmatrix} I & O \\
-iH_1 & -H_2 \end{pmatrix}.$$ \(14\)

The total transfer matrix can be constructed by multiplying all transfer matrices corresponding to each layer and applying appropriate boundary conditions across each interface. That is

$$T = \prod_{i=1}^{l-1}P_i^{-1}B_i^{-1}B_iP_i e^{D_i\Delta z_i},$$ \(15\)

where $P_i, B_i, D_i$ and $\Delta z_i$ are the eigenvector matrix, boundary condition matrix, eigenvalue matrix and length of the $i$th layer. Also $l$ is the number of layers (here $l = 3$). As can be traced, the total transfer matrix will depend on system energy, i.e. $E$. In order to determine the permitted energies, wavefunction normalization should be considered.

Referring to figure 1, if $a_i$ and $b_i$ denote forward and backward wave vectors, respectively, at the interface between $i$th barrier and well, the following should hold for bound states, when $a_1$ is set to zero

$$a_2 = T_{11}(E)a_1 + T_{12}(E)b_1 = T_{12}(E)b_1,$$

$$0 = T_{21}(E)a_1 + T_{22}(E)b_1 = T_{22}(E)b_1.$$ \(16\)

So particular $E$ is the system eigenenergy or equivalently the system has a non-trivial bound state, if and only if $T_{22}$ has an eigenvalue equal to zero for that specific $E$. In order to find the eigenvalues, the energy $E$ can be swept while the determinant of $T_{22}$ is monitored. In figure 2 the outcome is depicted for a specific $k_1$ near $\Gamma$ point in the reciprocal lattice.

The only problem involved with the above-mentioned approach is the appearance of spurious states. This is probable because such a procedure is a perturbative, in which an incomplete basis set is used. These spurious states reveal themselves in a rather large eigenvalues of $\Lambda$ for some layer and hence may result in instability. This problem can be treated by eliminating such eigenvalues in the $D$ matrix or clamping them appropriately.

Figure 2 shows three zero-crossing points in the swept range of energy, hence the system has at least three bound states. Note that for the sake of illustration two scales for the vertical axis have been used. Also the corresponding
eigenvector, i.e. \( b_1 \), can be evaluated for these three zero-crossing points, as shown in figure 3.

As the matrix elements of the Luttinger Hamiltonian in (7) are written in a symmetric basis other than pure \( \pi \) orbitals, i.e. \( p_x \uparrow, p_y \downarrow, p_x \downarrow, p_y \uparrow, p_z \uparrow \) and \( p_z \downarrow \), the resultant envelope wavefunctions \( b_1 \) are not symmetric with respect to the \( z = 0 \) plane. Here, a unitary transformation is employed in order to symmetrize these envelope wavefunctions. In figure 3, the normalized six envelope wavefunctions \( p_x \uparrow, p_y \downarrow, p_x \downarrow, p_y \uparrow, p_z \uparrow \) and \( p_z \downarrow \), for the first bound state are depicted. It can be seen that the contribution of these envelope functions in total wavefunction is not identical. By investigating similar curves for other bound states it can be realized that the most significant envelope functions vary with respect to the bound state under consideration.

The matrix representation of the exciton Hamiltonian operator, i.e. \( \hat{H}_X' \), is attained by projecting it on the space spanned by vectors obtained from the tensor product of electron and hole Hamiltonian eigenvectors

\[
\hat{H}_X' = \langle \psi' \rangle \hat{H}_X |\psi' \rangle, \tag{17a} \\
|\psi' \rangle = |\psi'_e \rangle \otimes |\psi'_h \rangle. \tag{17b}
\]

The dimension of this matrix depends on the number of bases taken into account. Considering the exciton Hamiltonian in (1), one can recognize that in contrast with the first two terms, the third term, i.e. the Coulomb interaction term, results in integrations in a six-dimensional space as the exciton Hamiltonian matrix elements are asked to evaluate.

Evaluation of such high dimensional integrals is computationally expensive, so we used an IPM cluster computer equipped with the LAM-MPI library [41, 42]. Furthermore, we used the VEGAS integration algorithm in order to increase the convergence rate [43, 44]. The exciton Hamiltonian matrix representation is obtained by incorporating a basis set consisting of 243 \((3^5 = 243)\) vectors.

Figure 3. (a)–(f) Envelope wavefunctions obtained for the first bound state correspond to \( p_x \uparrow, p_y \downarrow, p_x \downarrow, p_y \uparrow, p_z \uparrow \) and \( p_z \downarrow \) Bloch parts, respectively.

Figure 4. Spectrum of exciton energy obtained through matrix diagonalization. Each blue line denotes an exciton state.

The number of bases depends on the chosen maximum of the six quantum numbers, i.e. \( n, \nu, d, m, \omega \) and \( b \). If we consider only bound states in the \( z \)-direction, one can set \( d_{\text{max}} = 1 \) and \( b_{\text{max}} = 3 \) owing to the limited height of potential barriers in that direction for both electron and hole. Other quantum numbers correspond to the in-plane discretizations which have finer effect on energy distribution compared to \( b \) and \( d \). That is why the QD radius is an order of magnitude bigger than its thickness. Also, \( n_{\text{max}}, m_{\text{max}}, \omega_{\text{max}} \) and \( \nu_{\text{max}} \) have been set to 3. This choice can contain more bases at the cost of more computation burden, but yield negligible refinement for our purpose. Since the exciton Hamiltonian is Hermitian, we needed to evaluate only 29646 matrix elements. In figure 4, the calculated spectrum of exciton Hamiltonian eigen energies is shown from direct diagonalization of its matrix representation. Also the \( A_{\nu, \omega} \) coefficients in (3) are obtained through this analysis by evaluating the corresponding eigenvectors.

3. Photonic crystal cavity

In order to have a strong coupling between an exciton and a photon, one needs to trap the photon in a rather high quality factor cavity, from which a photon cannot escape easily. PhC-based cavities seem to be the best solution thanks to their unique abilities to manipulate light. There are several papers published in designing high quality factor PhC-based cavities [19, 21, 45–48]. Although the 3D-PhC cavities are more effective in light trapping, 2D-PhC slab cavities are easier to fabricate, and we therefore will deal with such 2D-slab configurations.

We are interested in a high quality factor TE-like mode with a small mode volume. The micromachined cavity is formed by introducing a point defect in a perforated air hole triangular PhC slab depicted in figure 5.

In such structures, total internal reflection and Bragg reflection are the two mechanisms responsible for light localization in the out-of-plane and in-plane directions, respectively. In this structure, delocalization and cancellation
mechanisms can be applied to decrease the vertical losses [49–51]. Since the structure is symmetric with respect to $z = 0$ plane, TE-like and TM-like modes are available. Also the TE gap occurs between two lowest bands. Choosing slab thickness and air hole radius in the range of $0.5a < d < 1.2a$ and $0.35a < r < 0.4a$ respectively, yields a relatively large gap over a mid-gap ratio. In our design, we set $d = 0.71a$ and $r = 0.37a$ which results in opening a gap between the normalized frequencies 0.2574 and 0.3911.

The defect modes frequencies are obtained through finite-difference time-domain (FDTD) analysis by exciting the cavity with a broadband electric dipole having bandwidth equal to the PhC band gap. Yee’s algorithm is employed to implement FDTD [52]. We will focus on a symmetric mode both with respect to $x = 0$ and $y = 0$ plane which has the lowest frequency. Furthermore, the radius of nearest air holes is set to $0.3a$ in order to achieve a relatively high quality factor as well as a small mode volume [21]. The increase in the quality factor by changing the radius of the nearest holes is owing to the redistribution of the spatial Fourier components, i.e. in $k$-space, of the cavity-mode electric field. In fact this trick results in pushing the Fourier components out of the light cone and hence reducing the vertical radiation losses.

The corresponding Q-factor is estimated by exciting the cavity with a narrowband electric dipole centred at the mode resonant frequency and monitoring the electric field decay at a low symmetric point after the input is switched off. The frequency and time domain responses as well as the mode spatial profile are depicted in figure 6.

For obtaining reasonable results, Split-PML absorbing boundary condition is applied at the top and bottom layers each shifted about $0.5a$ into air, i.e. $c$ is set to $0.5a$ [53]. Also four periods in each direction are employed and seem sufficient. The grid is set to 20 cells per lattice constant, and subpixel smoothing is employed for better accuracy [54].

The Q-factor and normalized resonant frequency are evaluated as about 14 000 and 0.298, respectively, for the probed mode. Note that the experimental cavity Q-factor is expected to be slightly lower than that of the simulated one due to other loss mechanisms such as material absorption and scattering from fabrication imperfections. We will choose the PhC lattice constant, $a$, such that the exciton and photon
frequencies are in resonance. Also, the PhC mode Q-factor can be used to approximate the density of states when system time evolution is under consideration.

4. Exciton–photon interaction

In this section we investigate the interaction between an exciton and a photon residing in the aforementioned QD and PhC cavity, respectively. We will limit ourselves by supposing only one photon resides in the cavity. The Hamiltonian governing the system consists of an exciton and a photon can be simplified by using rotating wave approximation (RWA), i.e. supposing energy conservation holds during interaction. In the case of the exciton–photon Hamiltonian, we will exploit the second quantized form and field operators in order to work in a consistent mathematical framework. The total Hamiltonian reads

\[ \hat{H} = \hat{H}_X + \hat{H}_E + \hat{H}_L, \]

\[ \hat{H}_X = \sum_p E_p u_p^\dagger u_p, \]

\[ \hat{H}_E = \sum_k \hbar \omega_k c_k^\dagger c_k. \]

Here, \( E_p \) and \( \omega_k \) denote the exciton energy at level \( p \) and the photon temporal frequency in \( k \)th mode, respectively. Also \( c_k^\dagger \) and \( c_k \) are the bosonic creator and annihilator of photon at \( k \)th mode satisfying the commutation relationship \( [c_k, c_k^\dagger] = 1 \), respectively. Similarly, \( u_p^\dagger \) and \( u_p \) stand for the fermionic creator and annihilator of an exciton at level \( p \) satisfying the anticommutator relationship \( [u_p, u_p^\dagger] = 1 \). Based on (3), it is straightforward to observe that

\[ u_p^\dagger = \sum_{O,L} A_{O,L}^p a_O^p b_L^\dagger, \]

\[ u_p = \sum_{O,L} A_{O,L}^p a_O b_L, \]

\[ |\psi^X_p\rangle = u_p^\dagger |0_X\rangle, \]

where \( a_O^p \) and \( b_L^p \) are creators of electrons and holes at the \( O \)th and \( L \)th levels, respectively. Here \( |0_X\rangle \) denotes the excitonic vacuum state in which there is no electron–hole pair.

Minimal coupling and direct coupling schemes are the two equivalent approaches for modelling of the interaction Hamiltonian [55]. Hereafter, we will assume a minimal coupling scheme. The interaction between a photon and an exciton may result in two physically distinct processes which should be dealt with separately: the process in which an exciton is created or annihilated, i.e. when an excitonic vacuum state \( |0_X\rangle \) is involved, and the process in which the exciton level changes. The former consists of an electronic transition from the valence to the conduction band, i.e. intraband transition, while the latter consists of only inter-band transitions of electrons and holes.

Regarding intra-band transition the interaction Hamiltonian will be linear in terms of excitonic and photonic field operators. In this case the interaction Hamiltonian reads

\[ \hat{H}_I = \sum_{p,k} g_{p,k} u_p^\dagger c_k + \text{H.c.}, \]

where \( g_{p,k} \) denotes the coupling coefficient between \( k \)th electromagnetic and \( p \)th excitonic states, and H.c. represents the Hermitian conjugate.

By exploiting the minimal coupling scheme and neglecting second-order terms which is justified in low intensity processes, the first quantization form of \( \hat{H}_I \) can be simplified as

\[ \hat{H}_I = \frac{e}{2m_p} \sum_{j=1}^N [\mathbf{A}(r_j) \cdot \mathbf{p}_j + \mathbf{p}_j \cdot \mathbf{A}(r_j)]. \]

The summation is over all unit cells in the QD semiconductor crystal, supposing there is only one electron per unit cell. Here, \( \mathbf{p}_j \) is the \( j \)th electron momentum operator while \( m_p \) and \( e \) are the electron rest mass and charge, respectively. Also, \( \mathbf{A} \) represents the vector potential operator given by

\[ \mathbf{A}(r) = \sum_k \sqrt{\frac{\hbar}{2m_0 \epsilon_k V}} (\mathbf{E}_k(r) c_k + \mathbf{E}^\dagger_k(r) c_k^\dagger). \]

Here, \( \mathbf{E}_k(r) \) is the \( k \)th mode spatial profile. By employing the dipole approximation as well as the RWA one can obtain the coupling coefficient as

\[ g_{k,p} = -i e \alpha_k^\dagger \sqrt{\frac{\hbar}{2m_0 \epsilon_k V}} \mathbf{E}(r_0) \cdot \mathbf{g}, \]

where \( \Psi \) stands for the envelope part of the wavefunction. The detailed derivation of the above relationship is given in the appendix.

As was mentioned in section 2, \( \chi \) is a linear combination of \( \pi \)-like orbitals for the hole wavefunction, and an \( S \)-like orbital for the electron wavefunction. It is common practice to employ experimental data to evaluate the above electric dipole moment matrix elements, because the involved Bloch parts are not exactly known for various semiconductor crystals. In the case of GaAs the matrix element \( \langle p | d | s \rangle \) is on the order of 30 Debye in which \( d \) stands for either \( x, y \) or \( z \) [56, 57]. Other matrix elements are zero owing to symmetry.

In contrast to intra-band transitions, the interaction Hamiltonian corresponding to the inter-band transition is bilinear in terms of excitonic field operators. In this case the second quantization form of the interaction Hamiltonian can be written as

\[ \hat{H}_I = \sum_{p,p',k} g_{p,p',k} u_p^\dagger u_{p'} c_k + \text{H.c.} \]

In this case, the coupling coefficients are defined through the following matrix element:

\[ g_{p,p',k} = \langle \psi_p^X | 0_X \rangle \hat{H}_I \langle \psi_{p'}^X | 1_k \rangle. \]

Again, exploiting the minimal coupling scheme and neglecting second-order terms, yields an expression similar to (21) as

\[ \hat{H}_I = \frac{1}{\sum_{w\in\{e,h\}} \epsilon_w} \sum_{w\in\{e,h\}} \frac{\epsilon_w}{m_w} \mathbf{A}(\mathbf{r}_w) \cdot \mathbf{p}_w + \mathbf{p}_w \cdot \mathbf{A}(\mathbf{r}_w). \]
where the summation is over the electron and hole from which an exciton is constituted. After substituting (26) and (22) into (25), the latter can be reduced to

\[
\begin{align*}
g_{p,p',k} &= g^c_{p,p',k} + g^b_{p,p',k} \\
g^c_{p,p',k} &= \frac{i e \hbar}{m_e^*} \sqrt{\frac{\hbar}{2 E_{0k} V}} E_k(r_e) \cdot \vec{g} \\
g^b_{p,p',k} &= \sum_{O,L,O'} A^V_{O,L} A^O_{O',L} \int \psi_e^O(r_e) \nabla_v^O(r_e) d^3r_e. 
\end{align*}
\]  

Again, the dipole approximation is employed. The counterpart equations for (27b) and (27c), i.e., for hole couplings, can be achieved by replacing \( e, L \) and \( O \) indices by \( h, O \) and \( L \), respectively. It is possible to further simplify the integrand by employing EFA and rewrite electron and hole functions in terms of corresponding envelope and Bloch parts.

In order to investigate the interaction phenomenon, we will simplify the total Hamiltonian (18a)–(18c) by considering only one excitonic state interacting with only one photonic mode. Furthermore, we assume that intra-band transition occurs during the interaction, and hence use the linear representation in (20). This gives

\[
\hat{H} = E_p \mu_p \hat{u}_p + h \omega_k \hat{c}_k + h g_{p,k} \hat{c}_k \hat{u}_p + H.c. \quad \text{(28)}
\]

Here the cavity mode has a finite Q-factor and hence a complex frequency. Henceforth \( \gamma_c \) denotes the full width at half maximum (FWHM) of the cavity mode.

Phenomenologically, the nonradiative exciton decay due to electron–phonon interactions can be included with a nonradiative linewidth, denoted by \( \gamma_X \), which allows the QD to be described via a complex frequency. This broadening is not radiatively limited, but is due to dephasing mechanisms, such as Coulomb interaction with free carriers [58]. The exciton nonradiative linewidth is on the order of few tens of \( \mu eV \) [59].

Considering these effects, one can find the Hamiltonian eigenenergies which read [60, 61]

\[
\begin{align*}
\omega^\pm &= \omega_0 - i \gamma_0 \pm \sqrt{g^2 - \left( \frac{\gamma_e - \gamma_X}{4} - \frac{i \Delta}{2} \right)^2}, \\
\omega_0 &= \frac{1}{2} \left( \omega_X + \omega_e \right), \\
\gamma_0 &= \frac{1}{4} \left( \gamma_e + \gamma_X \right),
\end{align*}
\]  

in which \( \Delta \) stands for detuning between exciton and photon states. When the coupling coefficient is large enough so that there are two eigenfrequencies with distinct real parts corresponding to two non-degenerate entangled states, the system operates in a strong-coupling regime. We set the PhC lattice constant to 244 nm so that the cavity mode under consideration be in resonance with the third exciton state, i.e., \( \Delta = 0 \) The corresponding energy is 1513.3 meV. Also the cavity-mode linewidth \( \gamma_c \) is calculated as 110 \( \mu eV \) equivalent to its quality factor. The QD is assumed to be located at the peak of photonic mode’s electric field profile in order to maximize the coupling coefficient. In order to have Rabi splitting, or equivalently for the system to be in the strong-coupling regime, it should have eigenfrequencies with distinct real values. Equations (29a)–(29c) indicate that when the cavity mode and exciton state are at resonance, the sufficient condition for the system to be in the strong-coupling regime is \( g^2 > \frac{1}{16} (\gamma_e - \gamma_X)^2 \). By using equations (23a), (23b) and the results obtained in section 3, the coupling coefficient is evaluated about 159 GHz. This predicts that Rabi oscillation will occur at \( 2 \sqrt{g^2 - \frac{1}{16} (\gamma_e - \gamma_X)^2} \) Hz.

5. Conclusion

In this paper, we studied the bound electron–hole pairs, i.e., excitons, quantum mechanically and used the Luttinger Hamiltonian in order to achieve their eigenstates in a disc-like QD precisely. We exploited these states to construct a basis set for the Hilbert space in which an exciton lives and use a matrix diagonalization method to approximate exciton eigenstates. Subsequently, a very high quality factor cavity has been designed by introducing a point defect in a triangular lattice photonic crystal slab. The coupling coefficient between photon and exciton states was examined and reformulated in order to inspect the interaction phenomenon. This phenomenon, in the field of quantum electrodynamics, quantum information and quantum computing has a variety of applications and plays a key role both in the weak and strong-coupling regimes. Finally, the numerical value of a coupling coefficient corresponding to a single exciton state and a high quality photon mode was evaluated and it was shown that the system is capable of operating in the strong-coupling regime.

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Appendix

In this appendix we will derive coupling coefficient expressions for intra-band transitions. The derivation of the coupling coefficient corresponding to inter-band transition is very similar. In the case of intra-band transition the interaction Hamiltonian is

\[
\hat{H}_i = \frac{e}{2m_e} \sum_{j=1}^{N} [A(r_j) \cdot \hat{p}_j + \hat{p}_j \cdot A(r_j)]. \quad \text{(A.1)}
\]

We substitute the momentum operator using \( \hat{p}_j = m_e [\hat{r}_j, H_j] \) and further simplify \( H_i \) by supposing \( [A(r_j), H_j] \approx 0 \), which is justified by assuming the dipole approximation. Hence, we get

\[
H_{\text{int}} = \frac{e}{i \hbar} \sum_{i=1}^{N} [\hat{r}_i, H_i] \cdot A(r_i) \quad \text{(A.2)}
\]
in which $H_e$ corresponds to interacting electrons in the semiconductor given by

$$H_e = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} - \sum_{i,l} \frac{Z e^2}{|r_i - R_l|} ,$$  \hspace{1cm} (A.3)

where $i$ and $l$ refer to the index of the electron and nuclei, respectively. Also, the quantized vector potential for photonic modes is

$$A(\mathbf{r}) = \sum_{\mathbf{k}} \sqrt{\frac{\hbar}{2\epsilon_0\omega_0}}(\mathbf{E}_k(\mathbf{r})c_\mathbf{k} + \mathbf{E}_k^*(\mathbf{r})c_\mathbf{k}^\dagger).$$  \hspace{1cm} (A.4)

By exploiting the two-band semiconductor model, one can write the many-electron ground state with the aid of the Slater determinant

$$|Y_0\rangle = A[\psi_{vk_1}, \psi_{vk_2}, \ldots, \psi_{vk_i}, \ldots, \psi_{vk_N}].$$  \hspace{1cm} (A.5)

Here, $A$ is the antisymmetrizing operator, $N$ is the number of unit cells, and $\psi_{vk}$ is the one-electron wavefunction corresponding to $\mathbf{k}$th electron in the semiconductor valence band. Also the exciton state at level $p$ can be written as

$$|Y_p\rangle = A[\psi_{vk_1}, \psi_{vk_2}, \ldots, \psi_{pX}^P, \ldots, \psi_{vk_N}].$$  \hspace{1cm} (A.6)

Note that $|Y_p\rangle$ is the eigenket of $H_e$ with eigenenergy $E_p$. The coupling constant is defined through the following matrix

$$g_{k,p} = \langle Y_p, 0 | \operatorname{H}_{\text{int}} | Y_0, 1^{\text{ph}} \rangle.$$  \hspace{1cm} (A.7)

It is straightforward to reduce (A.7) after substituting equations (A.2), (A.4) and (3) by using the bosonic creator and annihilator properties as

$$g_{k,p} = \frac{e}{\hbar} \sqrt{\frac{\hbar}{2\epsilon_0\omega_0}} \mathbf{E} \mathbf{g},$$  \hspace{1cm} (A.8a)

$$\mathbf{g} = \langle Y_p | \sum_{i=1}^{N} \mathbf{E}(\mathbf{r}_i) \cdot \mathbf{r} | Y_0 \rangle,$$  \hspace{1cm} (A.8b)

$$= \sum_{L, O} A^{P}_{L, O} \langle \psi_{k^L}^P \mathbf{E}(\mathbf{r}) \cdot \mathbf{r} | \psi_{k^O}^P \rangle.$$  \hspace{1cm} (A.8b)

Since the electric field profile has a large spatial wavelength compared to that of the electronic parts, one can ignore electric field variations and exclude them from integration. Upon using (EFA) in case of electronic wavefunctions, equation (A.8b) is further simplified as

$$g_{k,p} = -ie\omega^P_X \sqrt{\frac{\hbar}{2\epsilon_0\omega_0}} \mathbf{E}(\mathbf{r}_0) \cdot \mathbf{g},$$  \hspace{1cm} (A.9a)

$$\mathbf{g} \approx \sum_{L, O, i} A^{P}_{L, O, i} \langle \psi_{k^L}^P | \psi_{k^O}^P \rangle \langle \mathbf{x} | \mathbf{r} \rangle,$$  \hspace{1cm} (A.9b)

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