Electromagnetically Induced Exciton Mobility in a Photonic Band Gap

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(Received 9 March 2007; published 24 July 2007)

It is suggested that an exciton in the engineered vacuum of a photonic-band-gap–quantum-well heterostructure exhibits electromagnetically induced anomalous quantum dynamics. The exciton is dressed by coherent emission and reabsorption of virtual photons near the photonic band edge and captured in momentum space, lowering its energy by 1–10 meV and lowering its effective mass by 4–5 orders of magnitude. The photonic band gap simultaneously enables strong coupling to confined optical modes and long exciton lifetime.

DOI: 10.1103/PhysRevLett.99.046801 PACS numbers: 73.21.–b, 42.50.–p, 42.70.Qs, 71.36.+c

Photonic-band-gap (PBG) materials [1,2] are periodic dielectric materials in which light can be localized [3], in analogy to the electronic states in the band gap of a semiconductor. Inside a PBG, where spontaneous emission of light from atoms is suppressed [4–6], the resonance dipole-dipole interaction for energy transfer becomes the dominant interaction mechanism between atoms [7,8]. In this Letter, we suggest that this mechanism may dominate bound electron-hole (exciton) coherent transport in a PBG. We demonstrate that a quantum-well (QW) exciton, suitably placed within a 3D PBG material, is strongly dressed by the emission and reabsorption of virtual photons, making it both a long-lived and ultramobile quantum excitation.

The study of excitons in semiconductor microcavities has a rich history [9–11]. However, the inability to simultaneously maintain long lifetime and strong optical coupling has been a fundamental impediment in the unambiguous observation of striking effects such as exciton Bose-Einstein condensation [12]. In this Letter, we show that the 3D PBG environment provides the possibility of simultaneous strong coupling between exciton and band-edge photons as well as the momentum-space capture of the exciton into a long-lived, low effective-mass, state. In particular, if the exciton recombination energy and in-plane wave vector coincide nearly with a photonic band edge, strong coupling effects provide up to a 10 meV reduction in the exciton energy. This leads to novel exciton dynamics and may facilitate quantum coherence of excitons, at up to 100 K, in the engineered electromagnetic vacuum.

We consider a heterostructure consisting of a QW sandwiched by woodpile [13] PBG material (see Fig. 1). The woodpile consists of rod stacks with a rectangular cross section. The width and height of the rods are 0.25a and 0.3a, respectively, where a is the lattice constant (the distance between two adjacent rods in the same layer). One unit cell of the woodpile consists of four stacking layers. Therefore, the vertical periodicity in the stacking direction is 1.2a. The QW thickness is chosen to be 0.06a.

Our proposed geometry for QW insertion consists of separating the two halves of a bulk PBG material by the thickness of the QW and then placing the solid semiconductor crystal layer in the resulting air gap. The intercalated thin quantum-well layer is ideally a high quality crystalline semiconductor made from well-studied III–V compounds, such as GaAs or InGaAsP. Recently, Noda et al. [14,15] have fabricated a closely related structure. Using a dielectric constant 11.9 for both the PBG material and the QW, we obtain the corresponding photonic band structure [Fig. 1(b)]. Two gray regions represent the original Bloch photonic modes of the bulk 3D PBG material without any defect. Two planar-guided bands [solid (red) lines] remain within the PBG. If the QW thickness is increased, more planar-guided modes enter the original 3D PBG. At a critical QW thickness of about 0.1a, the entire 3D PBG is filled with 2D guided modes. For 2D guided modes, the electromagnetic field is exponentially localized in the z direction and confined near the QW.

FIG. 1 (color online). (a) PBG-QW heterostructure, consisting of a QW layer of thickness 0.06a sandwiched by a woodpile structure. The dielectric rods have a rectangular cross section with width 0.25a and height 0.3a, where a is the center to center distance between adjacent rods in the same layer. (b) The photonic band structure consists of the shaded region (allowed bands in the 3D woodpile cladding region) and solid (red) curves (planar-guided modes induced by a QW defect). Labeled are (1) the planar band edge, (2) the upper 3D band edge, and (3) the lower 3D band edge.
Light in these modes can propagate only along the QW plane.

From our calculation of the planar-guided-band field patterns, using high resolution (50 points per lattice constant) finite-difference time-domain methods, we find that the QW layer screens the normal component of an applied electric field by acquiring surface polarization charges. In adapting the 3D band-edge modes to the QW layer, we assume that the only major modification of these modes to the QW architecture is a simple dielectric screening effect on the z component of the electric field. Because of the large dielectric constant of the quantum-well layer, the dominant contributions to the exciton-photon interaction come from larger, unscreened, in-plane electric field components of the Bloch modes.

The construction of a model Hamiltonian for exciton-photon coupling in a PBG environment is dictated by energy and momentum conservation considerations [16]. In a QW with continuous translational symmetry in the plane, momentum is conserved. This implies that an exciton with in-plane wave vector \( \vec{q} \) cannot undergo purely (one-photon) radiative decay unless it emits a photon with the same \( \vec{q} \). In general, this leads to the requirement for defects that act as recombination centers for radiative decay to occur. When the quantum well is sandwiched by 3D PBG material above and below, this continuous translational symmetry is replaced by the discrete translational symmetry imposed by coupling to Bloch mode photons. This discrete symmetry is characterized by the set of reciprocal lattice vectors \( \{ G_n \} \) for the 3D photonic crystal parallel to the QW plane. This implies that an exciton of wave vector \( \vec{q} + G_n \) can also recombine to emit a photon of wave vector \( \vec{q} \) in the 1st Brillouin zone of the photonic crystal. The QW breaks translational symmetry in the z direction. Consequently, a photon with arbitrary z component \( k_z \) can be emitted, provided such a photon exists near the recombination energy. A microscopic derivation of the exciton-photon coupling, taking into account the properties described above, will be presented elsewhere [17]. The resulting model Hamiltonian, parametrized by conserved quasi-momentum \( \vec{q} \) (under rotating wave approximation) can be written as

\[
H = H_{\text{exc}} + H_{\text{EM}} + H_{j},
\]

where

\[
H_{\text{exc}} = \sum_{j,n} E_{j,q} |j,n; q\rangle \langle j,n; q| + C_p^\dagger B_{j,q}^\dagger C_p |j,n; q| \langle j,n; q| + G_{q}^\dagger, \tag{1a}
\]

\[
H_{\text{EM}} = \sum_{p,k_z} \hbar \omega_{p,(\vec{q},k_z)} C_p^\dagger b_p |p,(\vec{q},k_z)| \langle p,(\vec{q},k_z)| + \text{H.c.}, \tag{1b}
\]

\[
H_j = \sum_{p,k_z} \sqrt{\hbar} g_{j,n,p} b_{j,q}^\dagger C_p |p,(\vec{q},k_z)| + \text{H.c.} \tag{1c}
\]

Here \( b_{j,q}^\dagger \) creates an exciton with the “bare” dispersion \( E_{j,q} \) (due to electronic hopping alone), for exciton polarization \( j \equiv (T, L, Z) \) and in-plane wave vector \( \vec{q} \) within the QW. These polarization states [11] arise from the different symmetries of atomic orbitals within the electronic unit cell of the microscopic electronic Bloch functions. \( C_p^\dagger |j,n; q\rangle \) creates a 3D Bloch mode photon in photonic band \( p \), with wave vector \( (\vec{q}, k_z) \) with frequency \( \omega_{p,(\vec{q},k_z)} \). The exciton-photon coupling constant \( g_{j,n,p} \)

\[
= -\left( \frac{e_{j,q} + C_p^\dagger}{\hbar} \sqrt{2 \hbar \omega_{p,(\vec{q},k_z)} \phi(0)} d_j u_{j,n,p} \right), \tag{2}
\]

with \( \phi(0) = 1.6 \times 10^8 \text{ m}^{-1} \) is the overlap amplitude in the electron and hole relative movement wave function, determined by the exciton Bohr radius. \( d_j \) is the magnitude of the \( j \equiv (T, L, Z) \)-exciton dipole. \( u_{j,n,p} \) is the Fourier component at \( \vec{q} + G_n^\dagger \) of the electric field in the \( j \) direction obtained from the photonic band edge \( p \) at the QW inserting position. Since we consider an exciton nearly resonant with a photonic band edge appearing at a certain wave-vector position, we attribute the field pattern at the band edge for the band \( p \) to the entire band \( p \) in approximating the coupling parameters \( \{ u_{j,n,p} \} \). Variations of these couplings at far away, off-resonant wave vectors make a negligible change to the final dressed exciton energies. The parameter \( l \) is the sample (quantization) length along the \( z \) direction for discretizing the electromagnetic modes. \( l \) is canceled out after performing integration over \( k_z \) for the final exciton renormalization. \( \epsilon_0 \) is the permittivity of free space. Since the bare exciton dispersion is negligible compared to the photonic dispersion, we simply set \( E_{j,q} = 0.8266 \text{ eV} \) (wavelength 1.5 \( \mu \text{m} \)). We have verified that realistic bare exciton dispersions have a negligible effect on the final dressed exciton mobility near band edges.

The dressed exciton eigenstate can be expressed as a linear superposition of bare exciton states and photonic Bloch modes, leading to a variational wave function in the Schrödinger picture:

\[
|\vec{q}\rangle_{\text{dressed}} = \sum_{j,n} C_{j,q} |j,n; q\rangle + G_n^\dagger |\text{bare}| + \sum_{p,k_z} C_{\text{phot}} (p, (\vec{q}, k_z))_{\text{photon}}. \tag{2}
\]

Here \( |j,n; q\rangle + G_n^\dagger |\text{bare}| \) represents a single bare \( j \)-exciton of wave vector \( \vec{q} + G_n^\dagger \) and zero photons. \( |p,(\vec{q},k_z)\rangle_{\text{photon}} \) represents a single photon in band \( p \) with wave vector \( (\vec{q},k_z) \) and no exciton. \( b_{j,n} \) and \( b_{\text{phot}}^\dagger \) are variational amplitudes of bare exciton eigenstates and the photons, respectively. This variational ansatz for the dressed exciton at wave vector \( \vec{q} \), denoted by \( |\vec{q}\rangle_{\text{dressed}} \), considers only contributions from the single exciton and single-photon sectors of the many-electron, multiphoton Hilbert space. \( E \) is the eigenenergy at a given \( \vec{q} \), giving rise to the dressed exciton dispersion. In what follows, we obtain a numerical solution for the variational (dressed exciton) energy for each \( \vec{q} \) within the photonic Brillouin zone. This is obtained by projecting the Schrödinger equation

\[
H|\vec{q}\rangle_{\text{dressed}} = E|\vec{q}\rangle_{\text{dressed}} \]

into the space spanned by the states \( |j,n; q\rangle + G_n^\dagger |\text{bare}| \) and \( |p,(\vec{q},k_z)\rangle_{\text{photon}} \). This yields the
coupled linear equations for the variational amplitudes:

\[ e_{j,\tilde{q}+G_0} b_{j,n}^{\text{exc}} + i\hbar \sum_{p,k_z} g_{j,n,p} b_{p,\tilde{q},k_z}^{\text{photon}} = E b_{j,n}^{\text{exc}}, \]  

(3a)  

\[ \hbar \omega_{p,\tilde{q},k_z} b_{p,\tilde{q},k_z}^{\text{photon}} - i\hbar \sum_{j,n} g_{j,n,p}^{*} b_{j,n}^{\text{exc}} = E b_{p,\tilde{q},k_z}^{\text{photon}}, \]  

(3b)  

Defining \[ A_p = \sum_{k_z} b_{p,\tilde{q},k_z}^{\text{photon}}, \] eliminating the amplitudes \[ b_{j,n}^{\text{exc}}, \] and performing a sum over \[ k_z, \] we obtain the eigenvalue condition:

\[ A_p = \sum_{j,n,k_z} -i\hbar g_{j,n,p}^{*}(i\hbar \sum_{p'} g_{j,n,p'} A_{p'})/(E - \hbar \omega_{p,\tilde{q},k_z}(E - e_{j,\tilde{q}+G_0})), \]  

(4)  

Equation (4) consists of \( p \) equations, one for each photonic band. Nontrivial eigenvalue solutions \( E(\tilde{q}) \) of this set of homogeneous, linear equations exist, provided that the determinant of the corresponding matrix of coefficients is zero. Because of the spatial mode orthogonality of different photonic band edges, they are nearly nonoverlapping on the QW plane [17]. We consider only one photonic band edge for each different exciton resonance. An exciton captured by a given band edge feels very little of the field of other band edges.

For an exciton interacting with the 3D upper photonic band edge, we obtain a stable exciton-photon bound state in the PBG. This new ground state appears as a local minimum in the dispersion of the dressed exciton. By setting the exciton recombination energy in resonance with the 3D upper band edge, we obtain the renormalized exciton dispersion in the first Brillouin zone shown in Fig. 2(a). The dispersion depth of the local minima is around 2.5 meV. An exciton, captured in momentum space by such a photonic band edge, becomes a highly stable and mobile entity with a renormalized effective mass of \( 10^{-4} \cdots 10^{-5} m_e \), \( m_e \) is the bare electron mass), comparable to the photon effective mass at the band edge.

The lower 3D band-edge photon dispersion in the first Brillouin zone exhibits maximal ridges where the photon in-plane effective mass is negative. However, at wave vectors \( \tilde{q} = (0, 0), (0.5, 0), (-0.5, 0), (0, 0.5), (0, -0.5) \), the photon effective mass is positive. When the bare exciton recombination energy is in resonance with the maximum lower band-edge frequency, the negative effective-mass ridges in the photon dispersion give rise to corresponding repulsive positive ridges in the renormalized exciton energy [see Fig. 2(b)]. However, these repulsive ridges lead to sharp local minima at other wave-vector positions with positive photon effective mass as mentioned above. Therefore, an exciton can be captured in these local minima. Depending on the specific PBG-QW heterostructure and choice of QW insertion position, the global minimum of the exciton dispersion could occur at any one of them. When the exciton is captured at \( \tilde{q} = 0 \), our numerical calculation shows that the renormalized exciton effective mass is about 3 orders of magnitude less than the electron mass.

For an exciton in near resonance with the 2D planar-guided-band edge, the relevant photons are localized in the \( z \) direction, and there is no need to perform the summation over \( k_z \), in the photon Hamiltonian (1b). This simplified Hamiltonian leads to the newly diagonalized eigenvalue branches referred to as the upper and the lower exciton polariton in analogy to the normal mode splitting of two coupled oscillators. A similar description has been used [10] for coupled exciton-photon mode splitting in a semiconductor microcavity. The resulting lower dressed exciton dispersion [Fig. 3(a)] exhibits local minima of 8.2 meV. The solid line in Fig. 3(b) shows how this magnitude varies as a function of the detuning between the bare exciton recombination energy and the 2D photonic band-edge frequency. This depth decreases with increasing detuning. The dashed line in Fig. 3(b) also shows the effective mass of the lower exciton polariton captured near the photonic band edge as a function of the detuning. Clearly, the effective mass remains about 4 orders of magnitude less than the electron mass over a significant range of detuning of the bare exciton from the 2D band edge. The resulting dressed exciton exhibits very high mobility.

In summary, we have demonstrated the possibility of anomalous exciton dynamics in a PBG-QW heterostructure, mediated by an engineered electromagnetic vacuum. Because of the PBG, single-photon radiative recombination is prohibited. Nevertheless, strong coupling is possible to slightly off-resonance band-edge photons. By emitting and reabsorbing virtual photons near the edge of the PBG,
the exciton dispersion acquires deep and sharp local minima in momentum space. This effect is most dramatic when the exciton wave vector and recombination energy coincide nearly with a photonic band edge. The exciton becomes strongly dressed and is captured by band-edge photon effective mass (4–5 orders less in magnitude of the bare electron mass). This high mobility, with a large effective de Broglie wavelength, leads to a spatial averaging over the potential arising from static disorder or phonons. This decreases the dressed exciton scattering by those potentials through a mechanism analogous to "motional narrowing" [18]. As the exciton effective mass become smaller, the rms scattering amplitude due to short-range-correlated disorder becomes proportionately smaller [17]. The transition matrix element for single phonon-assisted decay at very small $q$ is likewise very small [17,19]. Two counterpropagating longitudinal optical phonons may be required (simultaneously) for exciton decay. Coherence in the emission and reabsorption of virtual photons is likely to appear at temperature scales ($\leq 100$ K) defined by the depth of the dressed exciton dispersion minima, which in turn depend on the detailed photonic band structure. The renormalized exciton dispersion relation is almost independent of the original bare exciton hopping. This implies that our mechanism for dressed exciton dynamics applies not only to a QW layer but also to a layer of quantum dots placed within a 3D PBG material. The drastic decrease of the dressed exciton effective mass may facilitate observation of high temperature, many-body coherence effects, such as Bose-Einstein condensation [20]. The "half-light" nature of the dressed exciton also makes it promising for the development of low threshold lasers, in which the quantum statistics of emitted photons are governed by quantum correlations in the exciton many-body state [9].

We are grateful to Alongkarn Chutinan for helpful discussions. This work was supported in part by the Natural Sciences Engineering and Research Council of Canada, the Government of Ontario Premier’s Platinum Grant, and the Canadian Institute of Advanced Research.

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