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DG Angelakis, PL Knight & E Paspalakis

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Photonic crystals and inhibition of spontaneous emission: an introduction

D. G. ANGELAKIS, P. L. KNIGHT and E. PASPALAKIS

In the first part of this introductory review we outline the developments in photonic band gap materials from the physics of photonic band gap formation to the fabrication and potential applications of photonic crystals. We briefly describe the analogies between electron and photon localization, present a simple model of a band structure calculation and describe some of the techniques used for fabricating photonic crystals. Also some applications in the field of photonics and optical circuitry are briefly presented. In the second part, we discuss the consequences for the interaction between an atom and the light field when the former is embedded in photonic crystals of a specific type, exhibiting a specific form of a gap in the density of states. We first briefly review the standard treatment (Weisskopf–Wigner theory) in describing the dynamics of spontaneous emission in free space from first principles, and then proceed by explaining the alterations needed to properly treat the case of a two-level atom embedded in a photonic band gap material.

1. Introduction

At the microscopic level, ordinary matter exhibits behaviour analogous to light waves. When wave-like electrons scatter off ions in crystalline materials, constructive interference between different trajectories can cause electric currents to flow. Conversely, disorder in such crystals can hinder electrical conductivity, and for some energies the electrons become localized in space, thus preventing their free flow in the form of electrical currents. Although such ideas have been known since the 1960s, it is only recently that physicists have begun to ask whether similar effects can result in the localization of light in a corresponding 'photonic crystal'.

The purpose of this article is twofold. In the first part we outline the developments in photonic band gap (PBG) materials from the physics of photonic band gap formation to the fabrication and potential applications of photonic crystals. In the latter, we specifically focus on the state-of-the-art 3D structures exhibiting a full band gap in their

Authors' address: Centre for Quantum Computation, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Wilberforce Road, CB3 0WA, UK (DGA); QOLS, Blackett Laboratory, Imperial College, London SW7 2AZ, UK (PLK); Materials Science Department, School of Natural Sciences, University of Patras, Patras 265 04, Greece (EP).

electromagnetic field density of states, because as we believe, these are of great technological and fundamental interest. In the second part, we discuss the consequences for the interaction between an atom and the light field when the former is embedded in dielectric materials, mostly photonic crystals, which exhibit gaps in the density of states. We first review the standard treatment to describe the dynamics of spontaneous emission in free space and proceed by explaining the alterations needed to properly illustrate the dynamics of two-level systems embedded in a PBG material.

2. Developments in photonic crystals

2.1. From electrons to photons

A normal crystal is a periodic array of atoms which scatters and modifies the energy momentum relation of electrons, whereas a photonic crystal is an ordered inhomogeneous medium characterized by a spatially periodic dielectric constant, with the lattice parameter comparable to the wavelength of the light [1]. Figure 1 shows one such microstructure in which a complete bandgap at 1.5 μ m has been observed.

Strictly speaking, such a structure has no allowed electromagnetic (EM) modes in the forbidden range of frequencies

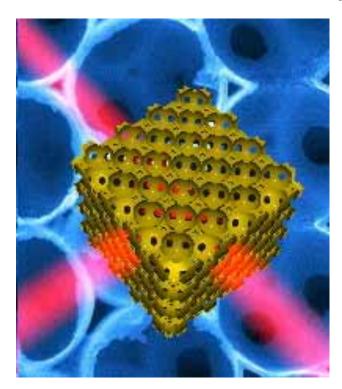


Figure 1. A 3D silicon photonic crystal exhibiting a complete band gap for incident light at 1.5 μ m. It is constructed by growing silicon inside the voids of an opal template of close-packed silica spheres which are connected by the small 'necks' formed during sintering, followed by removal of the silica template—see section 2 (courtesy of S. John's group, University of Toronto).

or in other words the density of states (DOS) of the propagating photon modes is zero (see figures 2 and 3). By contrast in free space (a cavity of infinite volume) the density of modes varies as ω^2 and exhibits no gap. In a cavity of finite volume the density of states is substantially modified for frequencies close to the cavity cut-off. Below the cut-off the cavity sustains no modes at all, and just above the cutoff, the density of states can be increased to the continuum case. The vanishing of the density of propagating photon modes within a PBG means that, for the frequency range spanned by the gap, linear propagation of electromagnetic (EM) waves is forbidden in any direction in the PBG material. Thus, light incident on a PBG material with a frequency from the gap region will be backscattered from the material, independent of the angle of incidence. Strong suppression of transmission with an associated peak in the reflectivity at the characteristic frequencies is then an experimental signature of a photonic band gap [2].

To give a further insight on the physics of light localization we will exploit the analogy between electron and light a bit further. As is well known an electron in a disordered solid is described by the following Schrödinger equation:

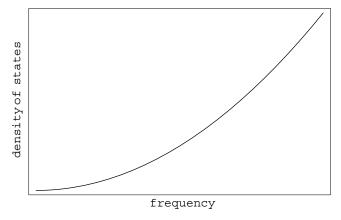


Figure 2. The density of modes of the EM field in free space.

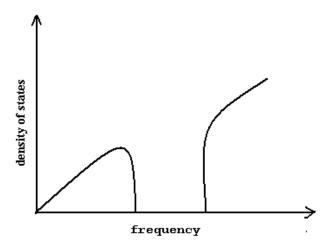


Figure 3. The density of modes of the EM field in a PBG structure with a broad gap.

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x}) = E\psi(\mathbf{x}) \quad , \tag{1}$$

where m^* is the electron's effective mass and $V(\mathbf{x})$ is a potential that varies randomly in space. For sufficiently negative energies E, the electrons may become trapped in regions where the random potential is very deep. The rate at which electrons tunnel out of the deep potentials depends on the probability of finding nearby potential fluctuations into which the trapped electron can tunnel. This rate increases as the electron energy increases.

In the case of a monochromatic EM wave of frequency ω propagating in an inhomogeneous but non-dissipative dielectric medium, the classical wave equation for the electric field is

$$-\nabla^2 \mathbf{E} + \frac{1}{c^2} \frac{\partial \mathbf{E}^2}{\partial t^2} = \mu_0 \frac{\partial \mathbf{P}^2}{\partial t^2} , \qquad (2)$$

where **P** is the polarization of the medium. Assuming now propagation in a linear medium, this leads to

$$-\nabla^2 \mathcal{E} - \frac{\omega^2}{c^2} \varepsilon_{\text{fluct}}(\mathbf{x}) \mathcal{E} = \varepsilon_{\text{D}} \frac{\omega^2}{c^2} \mathcal{E} , \qquad (3)$$

where \mathcal{E} is the slowing varying field amplitude. Also the total dielectric constant has been separated into its average value $\varepsilon_{\rm D}$ and a spatially fluctuating part $\varepsilon_{\rm fluct}(\mathbf{x})$. In a lossless material the dielectric constant $\varepsilon(\mathbf{x})$ is everywhere real and positive and plays a role analogous to the random potential $V(\mathbf{x})$ in the Schrödinger equation (see figure 4). It scatters the EM wave. Comparing now the above two equations (1) and (3) we observe the following differences. First, the quantity $\varepsilon_{\rm D}(\omega^2/\varepsilon^2)$ which plays the role of an energy eigenvalue, is always positive, which precludes the possibility of elementary bound states of light in deep negative potential wells.

Secondly the mode frequency ω multiplies the scattering potential $\varepsilon_{\text{fluct}}(\mathbf{x})$ and in contrast to an electronic system, where localization is increased by lowering the electron energy, lowering the photon energy leads to a complete disappearance of scattering. In addition, looking at the opposite high-frequency limit, geometric ray optics becomes valid and interference corrections to optical transport becomes less and less effective. These simply mean that in both cases the normal modes of the EM field are extended, not localized. Finally, the condition that $\varepsilon_D + \varepsilon$ - $_{\rm fluct} > 0$ everywhere translates into the requirement that the energy eigenvalue will always be greater than the effective potential $|(\omega^2/c^2)\varepsilon_{\text{fluct}}(\mathbf{x})|$. Therefore, unlike the familiar picture of electronic localization, what we are really seeking is an intermediate frequency window within the positive energy continuum that lies at an energy higher than the highest of the potential barriers. For those frequencies the interference between the incident and the scattered EM waves will be exactly destructive and this will allow no free propagating photon modes to exist in the structure [3].

In the following section, we quantify these ideas in a more rigorous way and present the procedure followed to find the allowed modes as a function of the frequency, the *dispersion relation*, in a simple 1D periodic dielectric.

2.2. Calculating the dispersion relation

The dielectric constant of any photonic crystal can be expressed as

$$\varepsilon(\mathbf{x}) = \varepsilon_{D} + \varepsilon_{fluct}(\mathbf{x})$$
 (4)

In this case we will assume that our structure exhibits periodicity in one dimension and is homogenous in the other two. More specifically

$$\varepsilon_{\text{fluct}}(x) = \sum_{n = -\infty}^{+\infty} u(x - nL) , \qquad (5)$$

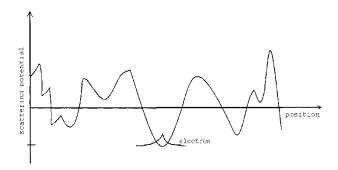
with L being the lattice constant and

$$u(x) = \begin{cases} n^2 - 1, & |x| < a, \\ 0, & \text{otherwise} \end{cases}$$
 (6)

As discussed in the previous section, the propagation of a monochromatic EM field in an inhomogeneous, nondissipative dielectric medium is governed by the following equation

$$-\nabla^{2} \mathcal{E} + \nabla(\nabla \cdot \mathcal{E}) - \frac{\omega^{2}}{c^{2}} \varepsilon_{\text{fluct}}(\mathbf{x}) \mathcal{E} = \varepsilon_{\text{D}} \frac{\omega^{2}}{c^{2}} \mathcal{E} , \qquad (7)$$

where \mathcal{E} is the field's ampitude. Setting $\varepsilon_D = 1$, the above equation reads $(\nabla \cdot \mathcal{E} = 0$, free charge is zero)



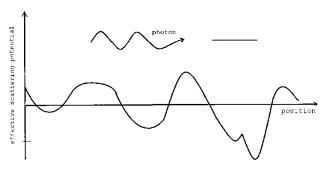


Figure 4. The scattering potential for electrons in a solid (top figure) and for photons in a random dielectric medium (bottom) [3]. The effective scattering potential for photons is $(\omega^2/c^2)\epsilon_{\rm fluct}$, where $\epsilon_{\rm fluct}$ is the spatially varying part of the dielectric. The electron (top) can have a negative energy and can be trapped in deep potentials. In contrast, the eigenvalue $(\omega^2/c^2)\epsilon_{\rm D}$ of the photon (bottom) must be greater than the highest of the potential barriers if the dielectric constant is to be real and positive everywhere.

¹All the dielectric materials described in this article will be assumed to be completely lossless.

$$-\nabla^2 \mathcal{E}(x) - \frac{\omega^2}{c^2} \varepsilon_{\text{fluct}}(x) \mathcal{E}(x) = \frac{\omega^2}{c^2} \mathcal{E}(x) . \tag{8}$$

Setting $\Phi(x) = -(\omega^2/c^2)\varepsilon_{\text{fluct}}(x)$ we obtain

$$-\nabla^2 \mathcal{E}(x) + \Phi(x)\mathcal{E}(x) = \frac{\omega^2}{c^2} \mathcal{E}(x) , \qquad (9)$$

where the potential $\Phi(x)$ is basically a sequence of 'potential barriers' of width 2a (see figure 5). The objective is to solve equation (9) for the potential $\Phi(x)$.

Restricting ourselves to a unit cell of the crystal, the solution can be expressed as follows

$$\mathcal{E}(x) = \begin{cases} A \exp(ikx) + B^{-ikx}, & x < -a, \\ C \exp(ik'x) + D \exp(-ik'x), & |x| < a, \\ E \exp(ikx) + Fe^{-ikx}, & x > a, \end{cases}$$
(10)

where $k = \omega/c$ and $k' = n\omega/c$. According to the Floquet theorem, E(x) should obey the following equation

$$\mathcal{E}(x+L) = \exp\left(ikL\right)\mathcal{E}(x) , \qquad (11)$$

and the derivative

$$\frac{\mathrm{d} \mathcal{E}(x+L)}{\mathrm{d}x} = \exp\left(\mathrm{i}kL\right) \frac{\mathrm{d} \mathcal{E}(x)}{\mathrm{d}x} \ . \tag{12}$$

In addition the boundary conditions are that both $\mathcal{E}(x)$ and $\mathrm{d}\mathcal{E}(x)/\mathrm{d}x$ should be continuous at $x=\pm a$. Applying all these conditions, we calculate the expansion coefficients and also the following transcendental equation describing the relation between ω and k:

$$\cos(kL) = \cos\left(\frac{2na\omega}{c}\right)\cos\left(\frac{b\omega}{c}\right) - \frac{n^2 + 1}{2n}\sin\left(\frac{2na\omega}{c}\right)\sin\left(\frac{b\omega}{c}\right), \tag{13}$$

which for b = 2na can be inverted analytically providing the *dispersion relation* for the 1D crystal,

$$\omega_k = \frac{c}{4na} \arccos \left[\frac{4n\cos(kL) + (1 - n^2)}{(1+n)^2} \right] . \tag{14}$$

This dispersion relation leads to gaps at $k = (m\pi)/[2(n+1)a]$ for odd integer values of m (see figure 6). The

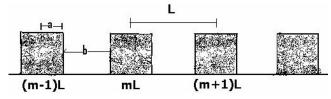


Figure 5. The periodic potential. L is the lattice constant.

lowest gap is centred at the frequency $\omega_{\rm gap} = \pi c/(4na)$ which for the case b = 2na equals π/L (case shown figure 5).

In the more general case of a realistic 3D photonic crystal, the usual approach is using the Bloch-Floquet theorem to expand both the field amplitude and the dielectric constant in plane waves whose wavevectors are reciprocal lattice vectors.

$$\mathcal{E}_{\omega}^{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G},l} b_{\mathbf{g},l} \mathbf{e}_{l} \exp\left[i(\mathbf{k} + \mathbf{G})\right], \qquad (15)$$

where \mathbf{e}_l is the polarization vector and \mathbf{G} are reciprocal lattice vectors. Using this expansion in equation (3), the problem is reduced to the solution of a system of linear equations on $b_{g,l}$ the solution of which provides the allowed mode frequencies for a given crystal (figure 7). We should

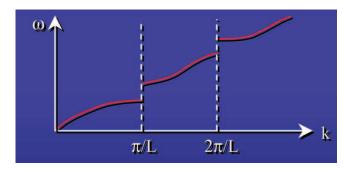


Figure 6. The dispersion relation for the 1D isotropic model shown in figure 5. As illustrated, gaps are formed at $m\pi/L$ for integer values of m.

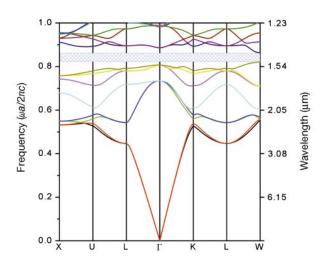


Figure 7. The band structure calculation of a realistic 3D photonic crystal (the inverse opal structure of figure 1) according to theoretical calculations. The shaded region corresponds to the gap predicted (width 5.1%) and partially observed by the Toronto group [4].

note here that for more complicated 3D structures the solution of the corresponding eigenvalue equation proves to be cumbersome and highly efficient computational techniques are usually required, see for example [5-11].

2.3. Fabrication of photonic crystals

In order to realize a 3D structure with a full band gap for the propagation of light for some specific frequencies, we need not only to show that a specific geometry could in principle exhibit a band gap but also that the specific microstructure is amenable to microfabrication in the lab [12]. To illustrate the methods followed by various groups in this field we will start with the simplest case, the traditional multilayer film. The latter is the simplest dielectric structure where one can observe inhibition of the linear propagation of an EM wave. It is relatively easy to construct by assembling together dielectric layers with alternating high and low refractive indexes.

To go further than that, i.e. to create a band gap in the propagation of an EM wave in two dimensions, we need something more sophisticated than simply contrast in the index of refraction. We need to find a specific geometry that will provide a full band gap for a range of frequencies in two dimensions. For this we need to keep in mind that the EM field consists of two types of modes. The transverse electric (TE) and transverse magnetic (TM) ones. To achieve a complete band gap for all polarizations, the corresponding bands should not only exist but also overlap. TM band gaps are favoured in a lattice of isolated high index regions as in an array of dielectric columns in air. In contrast, TE band gaps are favoured in the inverse structure as in an array of air columns (veins) drilled in a dielectric substrate. Therefore to achieve a full band gap, we need somehow to reconcile these seemingly contradictory conditions [1]. A structure satisfying this, is a triangular lattice of low index columns (air) inside a high index medium (silicon), see figure 8. More specifically for the case where the radius of the columns is large enough, the spots between the columns behave like localized regions of high refractive index material and thus the above requirement should be satisfied. It was predicted that for r/a = 0.48 for the ratio between the radius of the air columns to the lattice constant, a complete photonic band gap should form exhibiting a gap-midgap frequency ratio of about 19%. The experimental verification was provided by Gruning et al. [13], who constructed the crystal using an electrochemical technique to etch out columns in a silicon substrate. Their subsequent measurements verified a band gap at $\lambda = 5 \ \mu \text{m}$.

However, to achieve complete inhibition of light in all directions, we need a 3D structure which exhibits periodicity in all three directions. Out of the plethora of different geometries, the one that was found, in theory

first [14] and experimentally later [15] to support a full 3D band gap is the diamond lattice.2 The structure initially suggested by the Iowa group consists of either dielectric spheres in air or air spheres embedded in a dielectric medium. Yablonovitch managed to implement the latter by mechanically drilling cylindrical holes through a dielectric block (with $n \sim 3.6$). The points where his tunnels coincided formed a diamond-like structure (see figure 9). In spite of the apparent simplicity and initial success of the method in demonstrating the existence of a band gap in the microwave region, the application of the same method for optical waves proved to be of great difficulty. In this case, the spheres and consequently the drill had to be in the micrometre region! We remind here that in order for the TM and TE gaps to overlap, both constituent materials (air and dielectric) have to be topologically interconnected and also a large contrast (at least 3) between the two is essential. These constraints limited the use of microengineering fabrication techniques (electron beam and X-ray lithography [16] which proved to be very successful in longer wavelengths.³

A different approach was the layer stacking technique proposed by Ho et~al. [17] (see figure 11) and implemented by Lin et~al. [18] where a gap at 1.5 μ m was reported and the seven layer crystal exhibited 1% transmission (it was believed to drop to 0.1% with ten layers). Along similar lines using a combination of electron beam lithography and reactive ion etching Noda et~al. managed to stack semiconductor rods with micrometre dimensions [19]. They reported 99.9% attenuation between 6 and 9 μ m using eight layers. We note here that both methods are promising for any large scale technological application (see next section) as they are characterized by low cost and high reliability.⁴

To overcome the difficulties of 3D sub-micron engineering it has also been proposed to utilize systems that tend to self assemble themselves into various geometries. The most promising one proved to be colloidal crystals and artificial opals. Colloidal particles have been synthesized by materials such as latex and SiO₂ in the range of a few nanometres to a few hundred micrometres. A suspension of colloidal microspheres, with a typical concentration of 10¹⁰ particles cm⁻³, can residue under gravity into a cubic-closed-packed structure with size of the order of 1 cm.⁵

²We note here that proposed common semiconductors such as silicon and germanium also follow diamond geometry.

³We note here the *ion drill* proposed by the Yablonovitch group which led to the fabrication of structures with band gaps in the near-infrared (1.1-1.5 μ m). The problem in this case was that only a few unit cells could be reliably produced.

⁴The MIT group led by Joannopoulos has recently proposed to build a 3D crystal by stacking 2D ones (see figure 10). They predict the opening of a full 3D band gap.

⁵Their crystalline structure resembles that of natural opals.

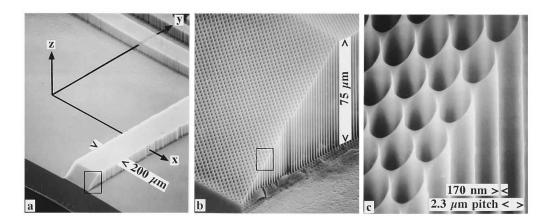


Figure 8. Macroporous silicon forming a 2-dimensional triangular lattice taken using scanning electron techniques [13]. (a) A porous silicon bar of width 200 μ m and height 75 μ m. (b) A tenfold magnification of the inset shown in (a). (c) A tenfold magnification of the inset shown in (b). The lattice constant of the macropore array is 2.3 μ m, the pore diameter is 2.13 μ m and the thinnest parts of the pore walls are 170 nm.

In spite of the advantage of producing inherently 3D structures [21] compared to the 2D ones using lithographic techniques, it appears to be extremely difficult to achieve the required refractive index contrast and interconnectedness for a full 3D band-gap to open. On the other hand, if they are used as templates to fabricate *inverse* opals (figure 1), i.e. cubic-closed-packed lattices of air bubbles on a dielectric matrix (silicon or GaAs) [4,22,23], near visible photonic band gaps with a gap to mid-gap frequency ratio of about 10% were predicted (see figure 7). We note here that the void regions that are left behind after the etching of the original template (Swiss cheese structure) will allow the injection of atoms or dye molecules thus making quantum optical type experiments possible. In spite of the initial success of the inverted opals in providing rather large band gaps in the infrared region, problems of gap instability to disorder effects may prove to be difficult to overcome. A solution to this was recently proposed by John's group at the University of Toronto [25]. They proposed an alternative photonic crystal architecture consisting of square spiral posts in a tetragonal lattice (figure 12). It seems that this structure could exhibit a quite large and robust 3D PBG occurring between the fourth and fifth EM bands and is also amenable to large-scale microfabrication using glancing angle deposition (GLAD) techniques. Spiral post lattices with microscale features have previously been synthesized using the GLAD method. In this technique, complex 3D structures can be fabricated by combining oblique vapour deposition and precisely controlled motion of a two-dimensionally patterned substrate. In addition, their square spiral posts can serve as templates for growing PBG materials from an even larger range of materials. In this case, a high refractive index

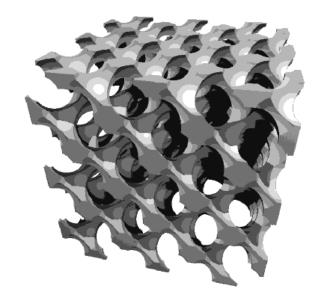


Figure 9. The first prototype structure predicted to exhibit a large and robust 3D PBG structure designed by Yablonovitch [15]. It consists of an overlapping array of air spheres arranged in a diamond lattice. It was created by drilling an array of criss-crossing cylindrical holes into a bulk dielectric of refractive index n = 3.6 where band gaps of the order of 20% were demonstrated. (Picture courtesy of the Toronto group).

material may be infiltrated to fill the void regions between the posts, with the posts subsequently removed by some selective etching process, leaving behind an 'inverted structure'. Their calculations have shown that the new

⁶In [24] a similar type of experiment for Bell Inequality testing is proposed.

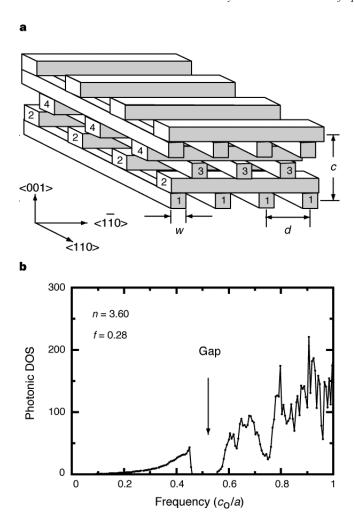


Figure 10. The woodpile structure fabricated by repetitive deposition and etching of multiple dielectric films. (a) Sketch of the layer-by-layer 3D photonic band gap structure. It is made from layers of one-dimensional rods with a stacking sequence that repeats itself every four layers, a unit cell, with a repeat distance of c. (b) Plot of the computer calculated photonic density of states assuming that the refractive index of the rods is n=3.60, the filling fraction of the 3D structure f=w/d=0.28 and c/d=1.414. A complete photonic bandgap exists from 0.46c/a to 0.56c/a, where c is the speed of light in vacuum [16].

inverted structure could exhibit an even bigger band gap which, for the case where the initial structure is infiltrated by silicon gaps, could be of the order of 27%.

2.4. Applications

One of the most immediate applications of photonic crystals was to be in optoelectronic devices where unwanted spontaneous emission affected their performance. On the left of figure 13 we show the electron dispersion relation for a direct gap semiconductor. Assuming that is embedded in a photonic crystal (whose photonic dispersion relation is



Figure 11. Computer reproduction of a novel 3D photonic crystal suggested by the Joannopoulos group [20]. The structure could be fabricated layer by layer following a three layer period thus allowing the use of traditional lithographic techniques, along with a high degree of control in placing defects (waveguides, cavities and other optical components) in the crystal. The layers consist of alternating stacks of the two characteristic types of 2D (or slab) photonic crystals: dielectric rods in air and air holes in dielectric.

shown on the right of the same graph) it is easy to see that if the PBG overlaps the electronic band edge then the electron—hole recombination rate could be inhibited. That is simply because the potentially emitted photon will have no place to go! In a semiconductor laser this would lead to near unity efficiency into the lasing mode. This theoretical idea was recently implemented [27] in the 2D band edge micro-laser in which lasing occurs preferentially at the 2D photonic band edge even though the emission from the active region has a broad frequency distribution (figure 14).

Along the same lines, light extraction from light-emitting diodes (LEDs) would be more efficient. The main problem there is that only the light emitted in a narrow angle⁷ manages to escape and the rest is usually trapped within the film and is either absorbed or emerges from the edge of the device. There are several ways to partially overcome this, for example using photon recycling, rough surface, etc., which could increase the efficiency to 30% but none of them actually alters directly the spontaneous emission properties of the device. If a 2D photonic crystal pattern in the form of a triangular lattice of air holes is introduced

⁷The efficiency being $1/(2n^2)$, where *n* is the index of refraction for the emitting material. For GaAs, n = 3.5 and the efficiency is approximately 5%.

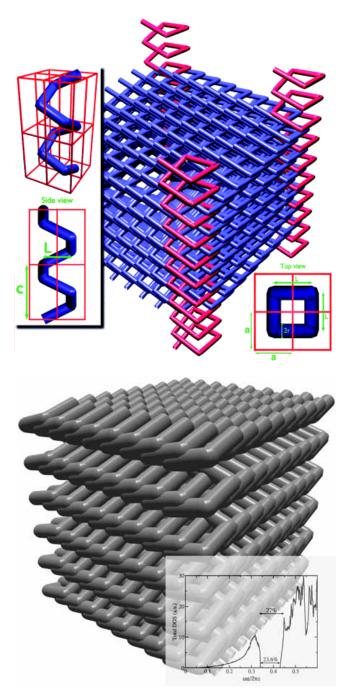


Figure 12. Top: the spiral crystal made of square spiral posts in a tetragonal lattice proposed by Toader and John. It is believed that structures like these might provide wider and more robust band gaps to disorder [25]. Bottom: The Si crystal obtained by inverting this template. A gap of 23.6% occurs between fourth and fifth bands of the photon dispersion relation. The corresponding total DOS is shown in the inset (arbitrary units).

into the semiconductor [31], extraction efficiency of the order of 100% is expected. This is simply due to the large band gap that will appear for in-plane propagation forcing the photons to come out of the slab in the vertical

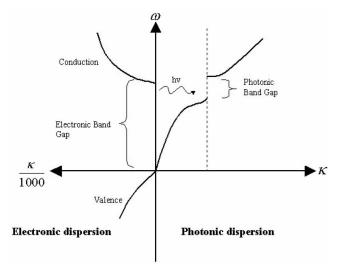


Figure 13. Diagram showing the dispersion relation for both the photon and electronic modes in a semiconductor integrated with a PBG material. The EM dispersion relation for the PBG structure is shown on the right whereas on the left is the electron wave dispersion relation typical of a direct gap semiconductor. If an electron for the conduction band were to recombine with a hole from the valence band and the PBG overlaps the electronic band edge, the resulting photon would not be emitted as there are no modes available there! This will result in the inhibition of the electron—hole recombination rate, seriously improving the performance of devices like semiconductor lasers as first suggested by Yablovonitch [26].

directions. In addition, unlike the planar microcavity, the efficiency is enhanced over a wide range of frequencies and as no resonance or photon recycling is needed, the photon lifetime is shorter. The latter of course leads to a reduction of the absorption losses and an increase of the modulation speed of the LED.

We proceed by describing the potential applications of the presence of defect modes in a photonic crystal. It was shown that by adding or removing a piece of dielectric material the periodicity of the lattice is locally altered and this can lead to the appearance of highly localized modes of light in an otherwise mode free surrounding. In particular, removing a small amount of high index material from one unit cell (air defect), leads to the occurrence of a localized mode just above the top of the lower band in analogy to the acceptor modes in semiconductors. On the other hand adding a small amount of high index material to a single unit cell (dielectric defect) forces a single localized mode to split off from the upper band edge as in semiconductor donor modes. The former case—an air defect—is basically a high-Q microcavity with tunable frequency. 8 All types of applications that involve high-Q optical microcavities thus

⁸The frequency of the defect mode is an increasing function of the volume of the defect area [1] and its energy is exponentially localized (usually within a few lattice constants).

could be implemented. The main advantage over usual high-Q superconducting metallic cavities is the operation on higher frequencies without almost any losses. Various devices such as frequency filters, atom masers, zerothreshold lasers should be more efficient (see figure 14 (b)). Also experiments involving single atom-photon interaction in the strong coupling regime is important and should be more easily realizable.

In a similar way to the introduction of point defects, someone can also create *line defects* in an otherwise perfect structure. Such defects could be used as lossless waveguides [33–37] where light could be guided around sharp corners with no reflection or scattering losses (see figure 15).

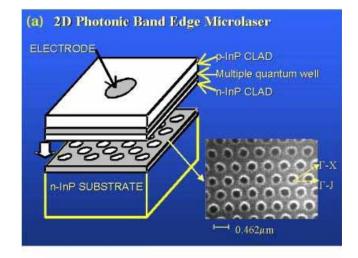
Last but not least, we mention the idea of creating tunable PBGs by the infiltration of inverted opal or spiral structures with some low index of refraction liquid crystal. The potential of controlling the direction of the nematic liquid crystal molecules through an external electric field, could alter the optical properties of the whole structure and simply provide external control over the width of a full 3D gap [38]. The resulting tunability of spontaneous emission, waveguiding effects and light localization may considerably enhance the technological value of a composite liquid crystal PBG material over and above that of either a bulk liquid crystal or a conventional PBG material by itself. A tunable optical microchip, which routes light from a set of optical fibres and could be used as part of a greater optical circuit, is shown in figure 16.

We conclude this part by noting that the intense interest in the field of photonic crystals in recent years has not solely been due to the above-described 'optical circuit' type of applications, where light was treated as a classical field. A lot of research has also been towards the understanding of the light-matter interactions within a photonic crystal at the quantum level. Several novel phenomena, such as, for example, the inhibition of spontaneous emission and the creation of 'atom-photon' bound states [39-66] and also the existence of transparency near a photonic band edge [67-71] were found in these studies. Describing the effect of inhibition of spontaneous emission and the creation of 'atom-photon' bound states will be the task of the next section.

3. Spontaneous emission

3.1. The influence of the reservoir

It was not until the 1980s [72] before it was established that spontaneous emission is not an intrinsic property of matter over which we have no control of [73] but a process greatly dependent on the nature of the surrounding environment.



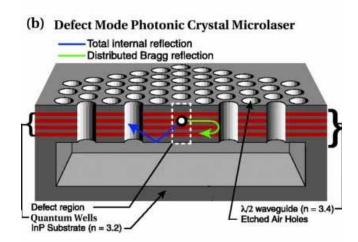


Figure 14. Designs for 2D photonic crystal micro-lasers. (a) The Band Edge micro-laser. Stimulated emission (arising from electron—hole recombination) from the multiple quantum well active region occurs preferentially at the band edge. It has been proved that strong feedback and memory effects can arise in this case [28]. For a real 3D case this would lead to lasing without a conventional cavity [29,30]. The Noda group has realized a precursor to this where broad frequency emission occurs preferentially at the band edge [27] (courtesy of S. Noda, Kyoto University). (b) Defect Mode micro-laser where a defect mode with a localized state of light within the 2D PBG structure is engineered by allowing for a missing pore in the 2D photonic crystal. Stimulated emission from the multiple quantum well active region falls mainly into the localized mode (courtesy of A. Scherer, California Institute of Technology).

We should note here that it was actually 1946 when an effectively overlooked paper by Purcell [74] already had suggested that the spontaneous emission rate of radiating dipoles can be tailored by using a cavity to modify the dipole-field coupling and the density of the available photon modes. If the modal density in the vicinity of the frequency of interest is greater than that of free space, then spontaneous

⁹It was experimentally shown [32] that the quality factor increases exponentially with the size of the crystal.

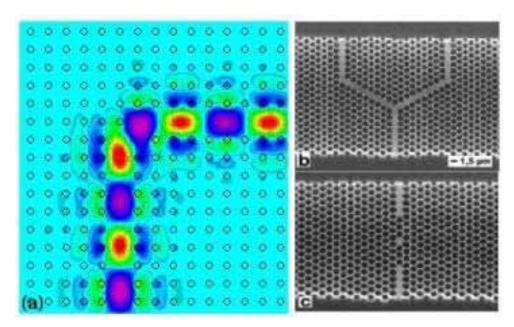


Figure 15. Waveguiding in photonic crystals. (a) Right angle waveguide channel in a 2D photonic crystal. The propagation of the field modes is through a line defect with no reflection or scattering losses (courtesy of J. D. Joannopoulos' group, Massachusetts Institute of Technology). (b) and (c) Other line defect microstructures fabricated in macroporous silicon with a lattice constant of 1.5 mm. The splitting of the modes in (b) could have application in building optical devices such as interferometers. In (c), the air holes within the line defect operate as reflectors or mirrors thus creating a resonator cavity within the waveguide (courtesy of Max-Planck Institute for Microstructure Physics, Halle, Germany).

emission will be enhanced, if it is less, it will be inhibited. This is the *Purcell effect*. Technological developments, in the form of high quality and finesse cavities, extended this to what we know today as cavity quantum electrodynamics (QED) [75]. One of the most characteristic concepts that was introduced at the time was the vacuum Rabi oscillations. To illustrate this, assume you have an atom, excited to some Rydberg state, placed inside a microwave cavity of high quality factor of the order of 10¹⁰ and mode spacing larger than the mode width. Assuming that the frequency of the transition from the initial Rydberg state to the nearest one matches one of the cavity modes, then spontaneous emission is greatly enhanced, whereas it is severely inhibited when the atomic transition is detuned from all cavity modes by an amount larger than the mode width. In the case of exact resonance, the spontaneously emitted photon is re-absorbed by the atom then re-emitted again and so on, leading to an oscillatory exchange of energy between the atom and the cavity radiation field. The operation of the micromaser is based on this effect where a constant exchange of coherent microwave photons between the mirrors of a microwave cavity and Rydberg atoms are flying through [76].

From the implementation point of view, the technological expertise required to built high-Q cavities has only recently moved from the microwave to the optical or near optical regime allowing for the possibility of similar research in the optical range [77]. The great obstacle in

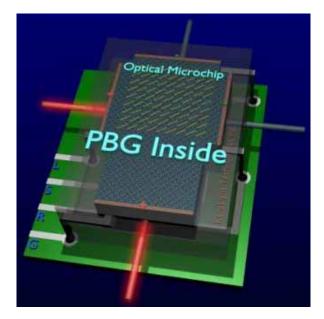


Figure 16. A futuristic depiction of an electro-actively tunable PBG routing device. The PBG structure has been infiltrated with an optically anisotropic material such as a liquid crystal (indicated by the yellow arrows) which responds strongly to external electric fields. Applying a voltage could alter the optical properties of the whole structure such that opening or closing of the corresponding photonic band gap could be achieved. This could lead to the possibility of routing light from an optical fibre into one of several output fibres (courtesy of S. John's group, University of Toronto).

localizing light in cavities is related to the shape of the cavity modes. Basically, there are always tails of the usual Lorenzian distribution of the cavity lineshape that extend to infinity allowing an excited atom located in the cavity to eventually decay to the ground state.

Extensive research in dielectric structures of the form described in the previous section showed that it was possible to fabricate situations where the modal density of the electromagnetic field exhibited gaps for a range of frequencies. As a qualitative approximation we would say that an excited atom tuned with the gap should never decay as there are no modes for its photon to exist. Initially led by John and collaborators and then quickly spreading to many groups throughout the world, an enormous amount of work has been produced dealing with questions usually asked in quantum optics, now extrapolated to PBGs, at least for their theoretical properties under somewhat idealized situations using the generalized density of modes for the PBG material [39-57,60,62-65] or under more involved situations where the local density of modes is used for the description of the PBG material [58,59,61,66]. The purpose of the following sections is to review some of the tools used in the above studies and more specifically in describing the dynamics of spontaneous emission. The first part describes the case where the atoms interact with the free space vacuum and the second with the structured continuum of a photonic crystal.

3.2. Two-level atom in free space: Weisskopf – Wigner theory

Suppose now we initially prepare our two-level atom in the upper state of the doublet and allow it to interact with the modes of the vacuum. The corresponding Hamiltonian, in the dipole and rotating wave approximations, is given by [78,79]

$$H = \hbar\omega_1 |1\rangle\langle 1| + \hbar\omega_2 |2\rangle\langle 2| + \hbar\sum_k \omega_k \beta_k^{\dagger} \beta_k + \hbar\sum_k (|2\rangle\langle 1|\beta_k g_{21}(\omega_k) + h.c.) ,$$
 (16)

where

$$g_{21}(\omega_k) = -\frac{\omega_{12}\mu_{21}}{\hbar} \left(\frac{\hbar}{2\varepsilon_0\omega_k V}\right)^{1/2} \hat{\varepsilon}_k \hat{\mu}_{21}, \tag{17}$$

and

$$\hat{\mu}_{21} = \int \phi_2(\mathbf{x}) e \mathbf{x} \phi_1(\mathbf{x}) d^3 \mathbf{x} , \qquad (18)$$

is the dipole moment for the transition $|1\rangle$ (lower state with wavefunction $\phi_1(\mathbf{x})$) to $|2\rangle$ (upper state with wavefunction $\phi_2(\mathbf{x})$). Here, β_k is the annihilation operator for the field mode k, V is the quantization volume and ε_0 is the electric

permittivity of free space. Also, $\hbar\omega_j$, j = 1, 2, is the energy of the *j*th atomic level. Finally, $\hbar\omega_k$ and $\hat{\varepsilon}_k$ denote the energy and the polarization vector of the *k*th reservoir mode, respectively.

Transforming the system in the interaction representation [78,79] we obtain the interaction Hamiltonian as

$$H^{(1)} = \hbar \sum_{k} |2\rangle \langle 1|\beta_k g_{21}(\omega_k) \exp \left[-i(\omega_k - \omega_{12})t\right] + h.c. ,$$
(19)

where $\hbar\omega_{12} = \hbar(\omega_2 - \omega_1)$. Assuming that initially the field modes are in the vacuum state $|0\rangle$, the wavefunction of the system can be written in terms of the state vectors as

$$|\psi(t)\rangle = a_2(t)|2,0\rangle + \sum_k b_k(t)|1,k\rangle , \qquad (20)$$

where the coefficients b_k represent probability amplitudes of emitting one photon of energy ω_k belonging to the vacuum modes $|1, k\rangle$ (with the atom in state $|1\rangle$). Also $a_2(t)$ represents the probability of the atom being in the excited state and the field has no photons. The time evolution of the system is described by the Shrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H^{(I)} |\psi(t)\rangle ,$$
 (21)

which using equation (19) leads to the following set of first order, coupled linear differential equations

$$i\dot{a}_2(t) = \sum_k g_{21}(\omega_k) \exp(-i\delta_k t) b_k(t) , \qquad (22)$$

$$i\dot{b}_k(t) = g_{21}^*(\omega_k) \exp(i\delta_k t) a_2(t) , \qquad (23)$$

where $\delta_k = \omega_k - \omega_{12}$ is the detuning of the emitted photon frequency from the atomic transition. We formally integrate equation (23) and obtain

$$b_k = -ig_{21}^*(\omega_k) \int_0^t a_2(t') \exp(i\delta_k t') dt' + b_k(0)$$
. (24)

Taking into account that $b_k(0) = 0$, we substitute equation (24) into equation (22) and obtain

$$\dot{a}_2(t) = -\int_0^t dt' a_2(t') \sum_k |g_{21}(\omega_k)|^2 \exp[-i\delta_k(t-t')], \quad (25)$$

which is still an exact equation. In order to proceed we have to calculate the kernel

$$K(t - t') = \sum_{k} |g_{21}(\omega_k)|^2 \exp\left[-i\delta_k(t - t')\right].$$
 (26)

The sum over modes is generally, converted to an integral, by including the density of modes (states) $\rho(\omega_k)$,

$$\sum_{k} |g_{21}(\omega_k)|^2 \exp\left[-\mathrm{i}\delta_k(t-t')\right] =$$

$$\frac{V}{(2\pi)^3} \sum_{\sigma} \int \mathrm{d}\Omega \int_0^\infty |g_{21}(\omega_k)|^2 \rho(\omega_k)$$

$$\times \exp\left[-\mathrm{i}\delta_k(t-t')\right],$$
(27)

where $d\Omega$ is the solid angle and σ is the light polarization. In free space, the product $|g_{21}(\omega_k)|^2 \rho(\omega) \sim \omega$ is a smooth varying function of ω . Taking this into account we can approximate

$$\int d\Omega \int_0^\infty |g_{21}(\omega_k)|^2 \rho(\omega) \exp \left[-i(\omega_k - \omega_{21})(t - t')\right]$$

$$\approx |g_{21}(\omega_{21})|^2 \rho(\omega_{21}) \int d\Omega \int_0^\infty \exp \left[i(\omega_k - \omega_{21})(t - t')\right],$$
(28)

which eventually gives [78,79]

$$K(t - t') = \frac{\gamma_{21}}{2}\delta(t - t')$$
, (29)

where $\gamma_{12} = \omega_{12}^3 \mu_{21}^2/(3\pi\epsilon_0\hbar c^3)$ is the famous free space decay rate. This approach is the much used Weisskopf–Wigner approximation.

The fact that the so-called response function K(t-t') is a delta-function means that the free space acts as an immediate response reservoir. In other words spontaneous emission is dealt with as a Markovian process and the evolution of the system depends only on the present and not on any previous state of the reservoir. Substituting equation (29) into (25) our initial set of equations become

$$\dot{a}_2(t) = -\frac{\gamma_{21}}{2} a_2(t) , \qquad (30)$$

$$i\dot{b}_k(t) = g_{21}^*(\omega_k) \exp(i\delta_k t) a_2(t)$$
 . (31)

The above equations can easily be solved with respect to time which gives

$$|a_2(t)|^2 = \exp(-\gamma_{21}t)$$
 (32)

3.3. Two-level atom in a photonic crystal

Assume now that our two-level atom is coupled to the radiation field of a modified reservoir. We will specifically assume that the atom is embedded in a three-dimensional photonic crystal where the photon dispersion is found to be an isotropic one and satisfies the following transcendental equation ¹⁰

$$\omega_k = \frac{c}{4na} \arccos \left[\frac{4n \cos (kL) + (1-n)^2}{(1+n)^2} \right].$$
 (33)

The Hamiltonian and the wavefunction of the system are still given by equations (19) and (20), and equations (22) and (23) still describe the evolution with the difference now that the atomic transition is occurring in the vicinity of a band gap in the density of allowed photon modes inside the photonic crystal. As we showed in the previous section the excited state amplitude a_2 is given by

$$\dot{a}_2(t) = -\int_0^t a_2(t')K(t-t')dt' . {34}$$

In order to calculate the kernel in this case we cannot use the Weisskopf-Wigner approximation as the density of states changes very rapidly in the vicinity of the atomic transition when located near the band edge. In this case, we must perform an exact integration in equation (26). To do this, we observe that in the vicinity of the gap the dispersion relation equation (33) can be approximated as

$$\omega_k = \omega_g + A(k - k_0)^2 , \qquad (35)$$

where $A \simeq \omega_{\rm g}/k_0^2$ (this corresponds to a density of states of the form $\rho(\omega) \sim \Theta(\omega - \omega_{\rm g})/(\omega - \omega_{\rm g})^{1/2}$ shown in figure 17, with Θ being the Heaviside step function [39]). The latter combined with equation (27) gives for the response function of equation (26)

$$K(t - t') = \frac{\beta^{3/2} \exp\{-i[\pi/4 + \delta_g(t - t')]\}}{[\pi(t - t')]^{1/2}}, t > t', \quad (36)$$

with $\beta^{3/2} = \omega_{12}^{7/2} |\mu_{12}|^2 / (6\pi\epsilon_0\hbar c^3)$ and $\delta_g = \omega_g - \omega_{12}$. Equation (36) demonstrates the non-Markovian character of the reservoir. In contrast to the free space case we can see from equation (36) that there is a contribution in the current dynamics at time t from previous states of the system at time t following an inverse square root dependence. As we will discuss later on, this is due to the partial localization of the emitted photon in the vicinity of the atom where it can be re-absorbed and thus affect the atom's evolution again after its initial emission.

We continue by trying to derive the explicit time dependence of the atom's evolution. To do that we need to solve the integro-differential equation (34). For this, we first Laplace transform it and obtain

$$s\tilde{a}_2(s) - a_2(0) = \tilde{k}(s)\tilde{a}_2(s)$$
, (37)

¹⁰We remind here that n is the refractive index of the scatterer, a is its radius and 2a + bL is the lattice constant (see section 2).

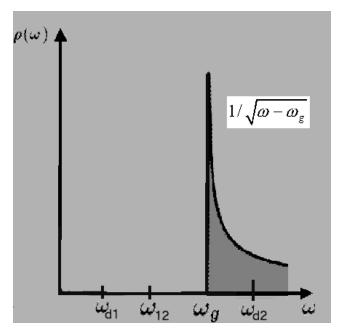


Figure 17. The density of states under consideration. ω_{12} is the atomic frequency and ω_{d1} , ω_{d2} the corresponding dressed state frequencies. These states emerge due to the 'self' dressing of the atom by its own localized radiation field.

where $\tilde{a}_2(s)$ and $\tilde{K}(s)$ are the Laplace transforms of $a_2(t)$ and K(t) accordingly. Using equation (36) we obtain for the excited state amplitude $\tilde{a}_2(s)$

$$\tilde{a}_2(s) = \frac{(s - i\delta_g)^{1/2}}{s(s - i\delta_\sigma)^{1/2} - (i\beta)^{3/2}} . \tag{38}$$

To obtain the dependence in the time domain we invert this using the Bromwitch formula:

$$a_2(t) = \frac{1}{2\pi i} \int_{\varepsilon - i\infty}^{\varepsilon + i\infty} \exp(st) \tilde{a}_2(s) ds , \qquad (39)$$

where the real number ε is chosen such that $s = \varepsilon$ lies to the right of all the singularities (poles and branch points) of the function $\tilde{a}_2(s)$. The inverse Laplace transform of equation (38) yields [41]

$$a_{2}(t) = 2b_{1}x_{1} \exp (\beta x_{1}^{2} + i\delta_{g}t) + b_{2}(x_{2} + y_{2}) \exp (\beta x_{2}^{2} + i\delta_{g}t)$$
$$- \sum_{j=1}^{3} b_{j}y_{j}[1 - \Phi((\beta x_{j}^{2}t)^{1/2})] \exp (\beta x_{j}^{2} + i\delta_{g}t) ,$$

$$(40)$$

where

$$x_1 = (A_+ + A_-) \exp(i\pi/4)$$
, (41)

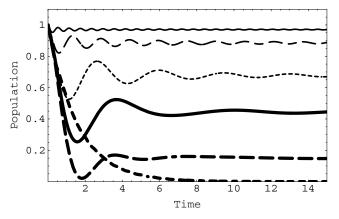


Figure 18. Atomic population on the excited state, $P(t) = |a_2(t)|^2$ as a function of time for various values of the detuning from the band edge: $\delta = -10\beta$ (thin solid curve), $\delta = -3.5\beta$ (thin dashed curve), $\delta = -1\beta$ (thin dotted curve), $\delta = 0$ (thick solid curve), $\delta = 1\beta$ (thick long-dashed curve) and $\delta = 10\beta$ (thick short-dashed curve). The time is in units of $1/\beta$.

$$x_2 = (A_+ \exp[-i(\pi/6)] - A_- \exp[i(\pi/6)] \exp[-i(\pi/4)],$$
(42)

$$x_3 = (A_+ \exp[i(\pi/6)] - A_- \exp[-i(\pi/6)]) \exp[i(3\pi/4)],$$
(43)

$$A_{\pm} = \left[\frac{1}{2} \pm \frac{1}{2} \left[1 + \frac{4\delta_{\rm g}}{27\beta^3} \right]^{1/2} \right]^{1/3} , \tag{44}$$

$$b_j = \frac{x_j}{(x_i - x_i)(x_i - x_k)} \quad (j \neq i \neq k; j, i, k = 1, 2, 3) , \quad (45)$$

$$y_j = (x_i^2)^{1/2} \quad (j = 1, 2, 3) ,$$
 (46)

and $\Phi(x)$ is the error function [80]. As we see from equation (41), if $\delta_g = 0$ then $\beta x^2_1 = i\beta$. This means that the value of β given above can be considered as a resonant frequency splitting, an analog of the vacuum Rabi splitting in cavity quantum electrodynamics [81]. For large times, i.e. for large values of βt , the terms of higher order than $(\beta t)^{3/2}$ [80] can be ignored, and equation (40) reduces to

$$a_{2}(t) \cong 2b_{1}x_{1} \exp \left(\beta x_{1}^{2} + i\delta_{g}t\right) + b_{2}(x_{2} + y_{2}) \exp \left(\beta x_{2}^{2} + i\delta_{g}t\right) + \frac{1}{2\pi^{1/2}} \left[\sum_{j=1}^{3} \frac{b_{j}}{x_{j}^{2}}\right] \frac{\exp \left(i\delta t\right)}{\left(\beta t\right)^{3/2}}.$$

$$(47)$$

As we see from equation (40) the atomic level splits into dressed states caused by the atom and its own radiation field located at the frequencies $\omega_{\rm d1} = \omega_{\rm g} - \beta {\rm Im}(x^2_1)$ and $\omega_{\rm d2} = \omega_{\rm g} - \beta {\rm Im}(x^2_2)$. It is easy to see using (41) and (44) that $x_1^2 = {\rm i}|x_1|^2$. This translates to the fact the correspond-

ing dressed state at the frequency $\omega_g - \beta |x_1|^2$ is the photon – atom bound dressed state with no decay. A photon emitted by the atom in this state will tunnel for a length scale of a few lattice constants before being reflected back and reabsorbed by the atom. The other dressed state conversely is pushed outside the gap, where the density of photon states is not zero and eventually will be responsible for the part of the initial excitation that will eventually decay (see figure 17). In figure 18 we show the atomic population as a function of time for various detunings from the band edge frequency. As was expected for atomic transitions well inside the gap ($\delta_g = -10\beta$), the atom remains in the excited state for ever. In this case the second term in equation (40) vanishes which means that no true atomic level splitting is present in this case and the oscillations in the dynamics are caused by the interference with a 'quasidressed' state originating from the branch point term. As $\delta_{\rm g}$ moves from negative to positive, the other component, located at $\omega_{\rm g}$ - $\beta |x_1|^2$ becomes important and eventually for $\delta_g = 10\beta$ is the major one forcing the atom to completely decay in the usual exponential manner. We note here that this photon atom bound state is present even when the atomic frequency ω_{21} is placed outside the gap where the density of states is not equal to zero and this is because of the special singular behaviour around the isotropic model there. For 'smoother' cases, such as smoothed models for the PBG density of modes or a Lorenzian density of modes, both the corresponding dressed states occur at complex frequencies which for long times leads to complete decay of the population to the ground state.

4. Conclusions

In this introductory review article we have discussed phenomena in photonic crystals with emphasis on the inhibition of spontaneous emission of atoms in such materials. We started by describing the physics behind photonic band gap formation by making a parallel with the known phenomenon of electron localization in solids and continued by presenting a simple model of a band structure calculation. We briefly presented the state of the art methods in fabricating photonic band gap materials. Some of the exciting applications in the field of optoelectronics were illustrated followed by noting the still theoretical but really exciting possibility of *circuits of light* in an all optical computing device. In the second part we moved to the quantum regime, i.e. the interaction of the quantized electromagnetic field inside a photonic crystal with small atomic systems. We discussed the way of treating the spontaneous emission of a two-level atom in free space using the Weisskopf-Wigner theory. We concluded this introductory review by presenting in detail the modification in the spontaneous emission of the same two-level atom when embedded in a photonic crystal of a specific type.

New phenomena arising by the localization of light as the complete *inhibition* of the spontaneous decay, *atom-photon bound state* and *population trapping* in a two-level atom were derived and discussed.

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Dimitris G. Angelakis is a Research Fellow of St Catharine's College, Cambridge, a position that he holds at the Centre for Quantum Computation in the Department of Applied Mathematics and Theoretical Physics, University of Cambridge. He was awarded his BSc degree and a MSc degree from the Physics Department, University of Crete in 1997 and 1998, respectively and his PhD from the Physics Department, Imperial College London in 2001. His research interests include studies in the areas of quantum optics, photonic crystals, CQED, Bell inequality tests, quantum information theory and quantum computation.

Emmanuel Paspalakis received a BSc degree and a MSc degree from the Physics Department, University of Crete in 1994 and 1996, respectively, and a PhD degree from the Physics Department, Imperial College London in 1999. After post-doctoral studies at the Physics Department, Imperial College London he joined the Materials Science Department, University of Patras in 2001, where he is currently a lecturer. His research contributions include theoretical studies in the areas of quantum optics, optoelectronics, dynamics of nanostructures and quantum computation.

Peter Knight is Head of the Physics Department at Imperial College London and has worked in quantum optics for many years. He was awarded his D Phil from Sussex University in 1972 following undergraduate studies at the same institution. He subsequently held research appointments at the University of Rochester and at Royal Holloway

before joining Imperial in 1979. He is the current President of the Optical Society of America, and Editor of the *Journal of Modern Optics* (and of *Contemporary Physics*).