

Spontaneous Radiation and Lamb Shift in Three-Dimensional Photonic Crystals

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Spontaneous emission in photonic crystals with anisotropic three-dimensional dispersion relation is studied. If the upper level is below a characteristic frequency ω_1 , or above ω_2 , or between ω_1 and ω_2 , the radiation is a localized field with a frequency in the band gap, or a propagating field with a frequency in the band, or a diffusion field, respectively. An analytical expression for the Lamb shift is obtained. The Lamb shift for the current case is small compared to that in an ordinary vacuum or in one- or two-dimensional photonic crystals due to lower density of states.

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There has been a growing interest in the study of periodic dielectric structures (photonic crystals) [1–5]. The inhibition of light wave propagation in photonic crystals provides a way to control spontaneous emission [4,5] that has many important applications [4]. The previous studies show that the gap edge has novel influences on optical behavior of an atom in a photonic crystal such as the appearance of photon-atom bound states [6–8], spectral splitting [9], enhanced quantum interference effects [8], coherent control of spontaneous emission [10], non-Markovian effects [6,11] etc. In these studies, the photonic crystal can be well represented by one band edge frequency ω_c and a dispersion relation. In many earlier studies, the photon dispersion relation near the band edge is assumed to be one dimensional [6–9,11]. A real photonic crystal in general has an anisotropic structure in momentum space, and a three-dimensional dispersion relation is required. The density of states (DOS) in a three-dimensional case is proportional to $(\omega_k - \omega_c)^{1/2}$ (ω_k is the frequency of the k th vacuum mode). In contrast, it is proportional to $(\omega_k - \omega_c)^{-1/2}$ in a one-dimensional case leading to a singularity. This may cause discrepancies as the density of states plays an important role in the interaction between light and materials.

In this paper we study how the spontaneous emission behaves if the three-dimensional dispersion relation is taken into account. The characteristics of the spontaneous radiation is considerably different from what is obtained in photonic crystals with one-dimensional dispersion relation. In particular, we find that there is no coexistence of a localized field and a propagating field. We also find a strong diffusion field that exists in the frequency domains where we have no localized and propagating field. These novel features are absent in crystals with isotropic dispersion relations [9]. Another important question pertains to the Lamb shift in the photonic crystals. It has been shown that the Lamb shift of a hydrogen atom in photonic crystals with one- and two-dimensional dispersion relations is different compared with that in an ordinary vacuum [6].

Because of an increased density of states, the Lamb shift of a two-level atom with its transition at the band edge for a photonic crystal with two-dimensional dispersion relation has been shown to be much larger than that in an ordinary vacuum [6]. This particular structure is very difficult to be manufactured. In this paper we calculate the Lamb shift of a two-level atom in photonic crystals with the three-dimensional dispersion relation.

Consider spontaneous emission from a two-level atom ($|a\rangle$ and $|b\rangle$) in a photonic crystal. In a photonic crystal, the vacuum dispersion relation is modified strongly by the periodic dielectric structures and an anisotropic band-gap structure is formed on the surface of the first Brillouin zone in the reciprocal lattice space. In general, the band edge is associated with a finite collection of symmetrically placed points \mathbf{k}_0^i leading to a three-dimensional band structure, for example, the eight L points on the surfaces of the first Brillouin zone of a diamond photonic crystal [1]. In the present study, the atomic transition frequency ω is assumed to be near the band edge ω_c . The dispersion relation for those wave vectors \mathbf{k} whose directions are near one of \mathbf{k}_0^i can be expressed approximately by $\omega_{\mathbf{k}} = \omega_c + A|\mathbf{k} - \mathbf{k}_0^i|^2$, where A is a model dependent constant. The Hamiltonian of the atom and the electromagnetic modes is

$$H = \hbar\omega|a\rangle\langle a| + \sum_k \hbar\omega_k b_k^\dagger b_k + i\hbar \sum_k [g_k b_k^\dagger |b\rangle\langle a| - \text{H.c.}]. \quad (1)$$

Here b_k (b_k^\dagger) is the annihilation (creation) operator for the k th electromagnetic mode with frequency ω_k , and $g_k = \frac{\omega d_1}{\hbar} \sqrt{\frac{\hbar}{2\epsilon_0 \omega_k V_0}} \mathbf{e}_k \cdot \mathbf{u}_d$ is the coupling constant between the k th electromagnetic mode and the atomic transition (assumed real). d_1 and \mathbf{u}_d are, respectively, the magnitude and unit vector of the atomic dipole moment.

The state vector of the system is given by $|\psi(t)\rangle = A(t)e^{-i\omega t}|a\rangle|0\rangle_f + \sum_k B_k(t)e^{-i\omega_k t}|b\rangle|1_k\rangle_f$, with the atom initially in the upper level. The state vector $|0\rangle_f$ describes

no photons existing in any modes, and $|1_k\rangle_f$ represents one photon in the k th mode. From the Schrödinger equation, we obtain the following equations for the amplitudes $A(t)$ and $B_k(t)$:

$$\frac{\partial}{\partial t} A(t) = - \sum_k g_k B_k(t) e^{-i(\omega_k - \omega)t}, \quad (2)$$

$$\frac{\partial}{\partial t} B_k(t) = g_k A(t) e^{i(\omega_k - \omega)t}. \quad (3)$$

Equations (2) and (3) can be solved by the Laplace transform method. The resulting expression for the amplitude is

$$A(t) = \frac{e^{x_1 t}}{F(x_1)} + \frac{e^{x_2 t}}{G(x_2)} - \frac{e^{i\delta\omega t}}{\pi} \int_0^\infty \frac{\beta^{3/2} i^{1/2} \sqrt{x} (\omega_c - ix) e^{-xt}}{[(\delta\omega + ix)(\omega_c - ix) - \sqrt{\omega_c} \beta^{3/2}]^2 - i\beta^3 x} dx, \quad (4)$$

where $\delta\omega = \omega - \omega_c$ and $\beta = [(\omega d_1)^2 (\sum_i \sin^2 \theta_i) / 8\pi \times \epsilon_0 \hbar A^{3/2}]^{2/3}$. In deriving Eq. (4), the summation over k is replaced by an integration over k . Because of the anisotropy, the integration over k has to be carried out around the directions of each \mathbf{k}_0^i separately. Here θ_i is the angle between the dipole vector of the atom and \mathbf{k}_0^i . The functions $F(x)$ and $G(x)$ are defined as $F(x) = 1 - x^2 / (2\beta^{3/2} \sqrt{-ix - \delta\omega})$ and $G(x) = 1 - ix^2 / (2\beta^{3/2} \sqrt{ix + \delta\omega})$. x_1 is the root of $x - i\beta^{3/2} / (\sqrt{\omega_c} + \sqrt{-ix - \delta\omega}) = 0$ in the region $[\text{Re}(x) > 0 \text{ or } \text{Im}(x) > \delta\omega]$, and x_2 is the root of $x - i\beta^{3/2} / (\sqrt{\omega_c} - i\sqrt{ix + \delta\omega}) = 0$ in the region $[\text{Re}(x) < 0 \text{ and } \text{Im}(x) < \delta\omega]$. The existence of x_1 and x_2 depends on the relative positions between the atomic frequency ω and the frequency of the band edge ω_c . If x_1 (or x_2) does not exist, the first (or second) term in Eq. (4) will be replaced by zero. There are three regions separated by two characteristic frequencies ω_1 and ω_2 (see Fig. 1), where we have different roots. $\omega_1 = \omega_c + \beta^{3/2} / \omega_c^{1/2}$ and $\omega_2 = 2\omega_c - \beta^{3/2} / [2\omega_c^{1/2} / 3 + (q_1 - q_2)^{1/3} - (q_1 + q_2)^{1/3}]$, with $q_1 = [(4\omega_c^3 - 20\omega_c^{3/2} \beta^{3/2}) / 27 + \beta^3]^{1/2}$ and $q_2 = 10\omega_c^{3/2} / 27 - \beta^{3/2}$. In region I ($\omega < \omega_1$) we have x_1 only (no x_2), in region II ($\omega_1 \leq \omega \leq \omega_2$) we have neither x_1 nor x_2 , and in region III ($\omega > \omega_2$) we have x_2 only.

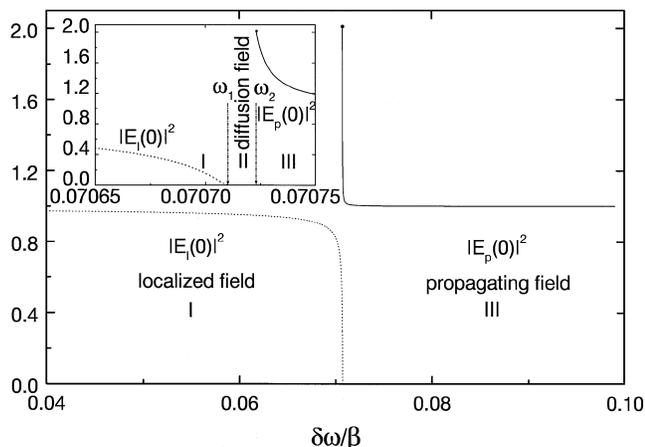


FIG. 1. The amplitude square (in arbitrary unit) of the localized mode and the propagating mode as functions of detuning of resonant frequency ω from photonic band edge with $\omega_c = 200\beta$ (the dotted curve is for the localized mode, and the solid curve is for the propagating mode).

The radiation $\mathbf{E}(r, t)$ can be obtained from $A(t)$ in a standard way [8,12]. The three terms in Eq. (4) yield three different emission fields. As x_1 is a pure imaginary root [8,9], the first field is a localized field near the atom. As x_2 is a complex root, the second field is a propagating field, which propagates out as a pulse with the energy velocity $\sqrt{A} \text{Re}(x_2) / \text{Im}(\sqrt{ix_2 + \delta\omega})$. The third field comes from the integration along the cut of the single valued branches and represents a diffusion field.

When the upper level is in region I ($\omega < \omega_1$), the radiation is composed of a localized field and a diffusion field. When the upper level gets into region II, the radiation consists of only a diffusion field. When the upper level is in region III, the radiation has a propagating field and a diffusion field. The diffusion fields in regions I and III are extremely small and can be neglected. However, it is very important in region II (see Fig. 2) (several hundred times stronger than in regions I and III) as all the energy is in this field.

From the above discussion the following picture emerges. The property of the radiation depends on the relative position of the upper level to the band edge. As the upper level moves from the gap to deep in the band, the radiation changes from mainly a localized field with a well-defined frequency less than ω_c to a mainly propagating field with a frequency larger than ω_c . During this process,

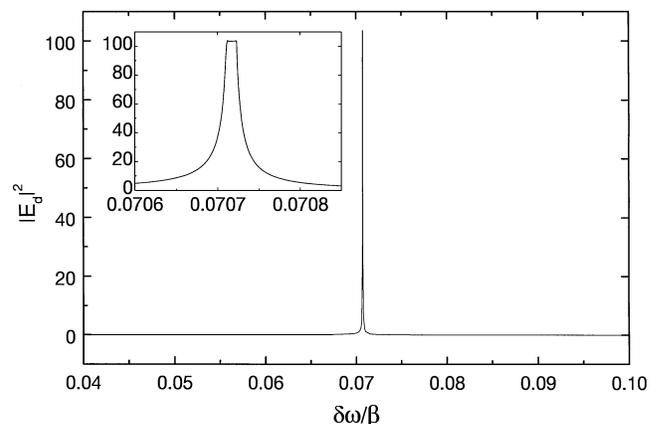


FIG. 2. The amplitude square (in arbitrary unit) of the diffusion field as a function of detuning of the resonant frequency ω from photonic band edge with $\omega_c = 200\beta$, $r\sqrt{\beta/A} = 1$, and $\beta t = 3$.

the diffusion field first increases while the localized field decreases. There is an energy transfer between the diffusion field and the localized field. Then the diffusion field decreases while the propagating field increases, i.e., the energy in the diffusion field is transferred to the propagating field.

In region I ($\omega < \omega_1$), the localized field can be expressed as $\mathbf{E}_l(r, t) = \mathbf{E}_l(0)e^{i(\omega_l - \omega)t - r/l}/r$. $\mathbf{E}_l(0)$ is a

ω dependent constant, $\omega_l = -ix_1$, and the size of the localized field is determined by the localization length, $l = [(-ix_1 + \omega_c - \omega)/A]^{-1/2}$. The localization length tends to infinity and the amplitude of the localized field tends to zero as ω goes to ω_1 .

In region II ($\omega_1 < \omega < \omega_2$; see inset in Fig. 1), there are no localized and propagating fields. The emitted field is a typical diffusion field,

$$\mathbf{E}_d(r, t) = \mathbf{E}_d(0) \frac{1}{r} e^{-i\omega_c t + ir^2/(4At) - i\pi/4} \int_0^\infty \frac{\beta^{3/2} \sqrt{x} (\omega_c - ix) dx}{[(\delta\omega + ix)(\omega_c - ix) - \sqrt{\omega_c} \beta^{3/2}]^2 - i\beta^3 x} \times \int_{-\infty}^\infty \frac{[ye^{3\pi i/4} + r/(2\sqrt{At})]e^{-y^2} dy}{-xt + i[ye^{3\pi i/4} + r/(2\sqrt{At})]^2}, \quad (5)$$

which carries all the energy. The evolution of $\mathbf{E}_d(r, t)$, with time t and the distance r from the atom, is shown in Fig. 3. As time t increases, $\mathbf{E}_d(r, t)$ at any space point increases first from zero to a maximum value, and then decreases to zero. Similar behavior can be seen considering $\mathbf{E}_d(r, t)$ as a function of the distance \mathbf{r} from the atom at a given time. The position of the maximum $\mathbf{E}_d(r, t)$ goes away from the atom with time (see Fig. 3). The spectral width is wide due to power law decay, and the energy diffuses out incoherently. This region is caused by the anisotropic dispersion relation and does not exist for an isotropic dispersion relation.

In region III, $\omega > \omega_2$, the dominant component of the emitted field is a propagating field. It has the form $\mathbf{E}_p(r, t) = \mathbf{E}_p(0)e^{i(\omega_p - \omega)t - \Gamma t/2 + iqr}/r$ with $\omega_p = \text{Im}x_2$, $\Gamma = 2\text{Re}x_2$, and $q = [(ix_2 + \omega - \omega_c)/A]^{1/2}$. This field propagates out coherently with all the energy (similar to the atom being in a vacuum). The behavior of $|\mathbf{E}_p(0)|^2$ is given in Fig. 1, indicating a pronounced switch-on ef-

fect for the propagating field when the sign of $\omega - \omega_2$ changes.

In the photonic crystal with the isotropic dispersion relation, a localized field and a propagating field can coexist [9,11]. However, this is not allowed in crystals with an anisotropic dispersion relation. This difference comes from the difference of DOS near the band edge in the two cases. There is a singularity in the isotropic case but not in the anisotropic case. In the isotropic case, any potential from an impurity (no matter how weak) will lead to localization [13] because of the singularity in DOS. This is why we always have the localized field in the isotropic case. In the anisotropic case there is no singularity in DOS, and the localization needs a potential larger than a certain value [13]. When the upper level moves up into the band from the gap, the frequency of the localized field approaches ω_c . In the isotropic case, the frequency of the localized field cannot be ω_c because of the infinite DOS at ω_c . An infinite DOS means infinite energy requirement for the localized field. In the anisotropic case, the frequency can be ω_c because the DOS is zero at ω_c , and when it is ω_c the localized field disappears (frequency larger than ω_c is in the band). At the same time the diffusion field (a field incoherently diffusing out) appears, but not a coherent propagating field because the number of electromagnetic modes near the atomic transition frequency is still not large enough. The further move of the upper level into the band will result in the propagating field with fixed phase. The sudden increase of the propagating field can be used to design an active optical microsized switch.

The Lamb shift of the atom is the difference between the frequency of the emitted field and the upper level frequency minus the contribution due to mass renormalization. The frequencies of the emitted fields are $\text{Im}(x_1)$ and $\text{Im}(x_2)$ for the localized and propagating fields, respectively. The frequency of the diffusion field is ω_c [see Eq. (5)]. The renormalization contribution is $\text{Im}(x')$ with x' being the root of $F'(x) = 0$, where $F'(x)$ is the same as $F(x)$ with ω replaced by zero [14]. Therefore we have the Lamb shift $\Delta_L = \text{Im}(x_{1,2}) - \text{Im}(x')$. In Fig. 4, we plot the

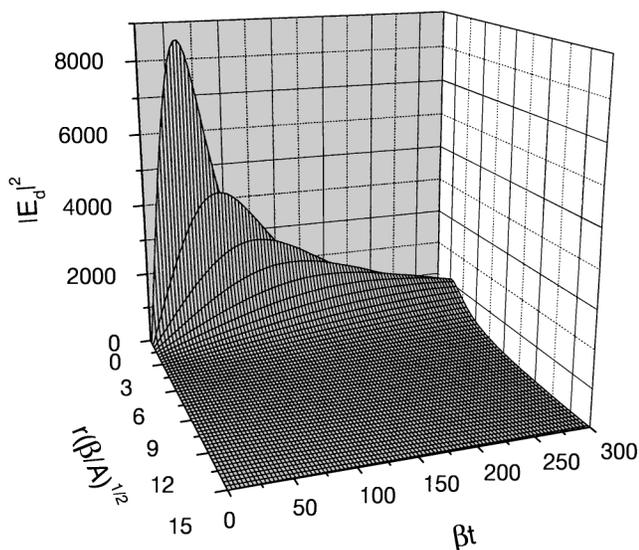


FIG. 3. The evolution of the diffusion field (arbitrary unit) with time and with the distance from the atom with $\omega_c = 200\beta$, $\omega = 200.07072\beta$.

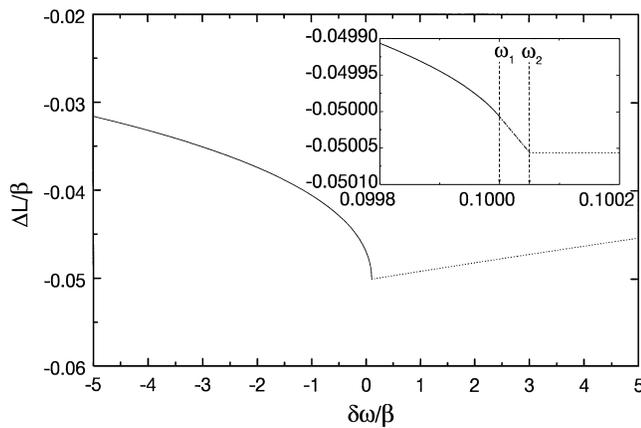


FIG. 4. The Lamb shift in unit β as a function of the detuning of atomic frequency from the photonic band edge $(\omega - \omega_c)/\beta$.

Lamb shift as a function of the atomic transition frequency $\omega - \omega_c$ for $\omega = 100\beta$. For $\omega = \omega_c$, the Lamb shift can be approximately expressed as $\Delta_L = -\beta/2\sqrt{\omega_c/\beta}$. If we let $\omega = 4 \times 10^{15}/\text{s}$ (green light) and a decay rate of $\gamma = 10^8/\text{s}$ ($\beta = \omega^{1/3}\gamma^{2/3} = 3.4 \times 10^{10}/\text{s}$), the Lamb shift is about $\Delta_L/\omega = 0.1 \times 10^{-7}$, which is smaller than that of $2S_{1/2}$ of a hydrogen atom in an ordinary vacuum. This is because the DOS in the photonic crystals with three-dimensional dispersion relations is much lower than that in the ordinary vacuum. This result is also very different from that from the one-dimensional case where DOS has a singularity, or from the two-dimensional case where DOS has a sudden jump [6].

In conclusion, the properties of the spontaneous radiation from a two-level atom in a photonic crystal strongly depend on the relative position of the atomic transition frequency ω to the band edge ω_c . The anisotropic dispersion relation results in two characteristic frequencies. Below these frequencies, the emission is mainly a localized field, whereas, above them, the emission is mainly a coherent pulse propagating out. For frequencies lying in between these characteristic frequencies, the emission is a diffusion field with all the energy diffusing out incoherently. The localized field and the propagating field cannot coexist. An analytical expression for the Lamb shift is obtained. The Lamb shift in anisotropic photonic crystals is less than that

in the ordinary vacuum or in crystals with one- or two-dimensional dispersion relations because of lower density of states.

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