Stimulated emission from an atom in a photonic crystal

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I analyze the stimulated emission process in photonic band structures. I consider a dipole transition of a two-level atom which is tuned near an edge of a photonic band gap. I solve numerically the Schrödinger equation for the chosen model without Born and Markovian approximations. It is shown that even one photon in the field can have significant influence on the dynamics of the system providing the atomic transition is tuned near sharp structures of the density of modes. [S1050-2947(99)09311-7]

PACS number(s): 42.50.Ct

One of the most fundamental processes in quantum optics is certainly stimulated emission (STE), i.e., a process when an excited atom interacts with a quantized electromagnetic field. If the initial field has a narrow spectrum (or if it is a classical field) its resonant interaction with the atomic transitions is also called resonant fluorescence (RF). A fully quantized treatment of the free-space RF is presented, for example, in Ref. [1] and in references therein. These authors analyzed STE to the first order in a fine-structure constant which can also be seen as a Markovian approximation. It was shown that the environment of photonic crystals can cause qualitative modifications of the spontaneous emission (SPE) [2-6] and other quantum-optics phenomena. Methods of exploring RF induced by a classical laser field were described for cavities [7] and photonic crystals [8,9]. In this Brief Report I analyze the STE from the atom when its particular transition is tuned near the band-gap edge (BGE). I consider the field in a fully quantized way. I assume that there is one photon prepared in the field at the initial time. The intent is to demonstrate the influence of the initial field on the dynamics of the atom-field system. Due to the abrupt variation of the density of the modes (DOM) at the BGE the interaction will be strongly modified in comparison with the interaction in free space. In particular, reversible energy exchanges between the atom and the field modes and the long-time memory effects contribute to the atom-field dynamics. This is a reason why in this case it may not be correct to perform Born and Markovian approximations. Therefore it may be convenient to use a direct integration of the Schrödinger equation. I restrict the calculations to systems with two excitations. I work within simplified models of the atom and the field (specified below), neglect light polarizations effects, and consider the atom at a fixed position. The conditions for the STE treated in this Brief Report are quite different from the conditions in Ref. [4].

I consider a two-level atom in a void region of a photonic crystal. The upper and lower atomic eigenstates are denoted as $|e\rangle$ and $|g\rangle$, respectively. In the initial time the atom is excited in its upper level. I consider the photonic band structure (PBS) with a continuous or quasicontinuous mode spectrum in the allowed bands. I assume that the initial electromagnetic field in the PBS is in a superposition of its one-photon states. Then the initial state of the system is a factorized product of the atomic upper state and the field superposition state,

$$|\Psi(0)\rangle = |e\rangle \otimes \sum_{\lambda} c_{\lambda}|1_{\lambda}\rangle.$$
 (1)

Here the vector $|1_{\lambda}\rangle$ describes the field modes in their vacuum states except the mode labeled by λ which is in Fock state with one photon. The exact form of the amplitudes c_{λ} will be specified below. I assume the interaction Hamiltonian in the dipole and rotating-wave approximations. In the Schrödinger picture the Hamiltonian reads

$$H = \frac{1}{2} \hbar \omega_A (1 + \sigma_z) + \sum_{\lambda} \hbar \omega_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} + \sum_{\lambda} \hbar (G_{\lambda} \sigma_+ a_{\lambda} + G_{\lambda}^* \sigma_- a_{\lambda}^{\dagger}) , \qquad (2)$$

where ω_A is the atomic transition frequency, ω_{λ} is the frequency of the mode λ , and G_{λ} is the coupling parameter between the atomic transition and the mode λ . The operators σ_{\pm} are atomic raising and lowering operators and σ_z is the atomic inversion operator.

I define the amplitudes c_{λ} by the relation

$$c_{\lambda} = \mathcal{N}\langle g, 1_{\lambda} | \exp\left(-\frac{i}{\hbar} H \tau_0\right) | e, \operatorname{vac} \rangle.$$
 (3)

In this expression H is the operator (2) (with parameters ω_A , ω_{λ} , and G_{λ} the same as considered in equations of motion for the STE). $|g,1_{\lambda}\rangle$ is the basis vector representing the atom in its lower level, the mode λ occupied with a single photon and all other modes in vacuum state. The basis vector $|e, vac\rangle$ represents the atom in its excited level and the field in the vacuum state. τ_0 is a suitably chosen parameter with the dimension of time and \mathcal{N} is a normalization constant so that $\Sigma_{\lambda} |c_{\lambda}|^2 = 1$. The values of c_{λ} can be relatively easily calculated numerically or also analytically for suitable models of DOM. (It is a task within the single-excitation subspace of the Hilbert space.) Here I calculate them numerically. For parameters considered in this Brief Report the energy of the field calculated from Eq. (3) is concentrated mainly to the modes near the BGE. At these conditions the light undergoes multiple reflections on the boundaries of the periodic PBS and it is very similar to a standing wave (see also the Footnote 2). For the given initial state (1) the following state vectors enter the dynamics of the system: $\{|e,1_{\lambda}\rangle, |g,2_{\lambda}\rangle, |g,1_{\lambda},1_{\lambda'}\rangle\}$, where $|a,n_{\lambda}\rangle$ represents the atom in its state $|a\rangle$ ($|e\rangle$ or $|g\rangle$), the mode λ occupied with n_{λ} photons, and all other modes empty. The vector $|g,1_{\lambda},1_{\lambda'}\rangle$

4183

describes the atom in its lower level, the two different modes occupied each with a single photon and all other modes empty. A similar problem was exactly solved by Davidson and Kozak [10]. In their final calculations they assumed that only one mode is initially occupied. They used the free-space DOM. A two-excitation problem (of superradiance) was exactly numerically solved also in Ref. [11]. Generally, dynamics with two excitations in a system given by the Hamiltonian (2) is difficult to solve analytically and even numerically. In this Brief Report I consider the STE using a qualitative model of the field and the interaction constants referred to as the "ideal" model. Firstly, I consider the DOM given by [4]

$$\rho^{\text{PBS}}(\omega) = K \frac{\sqrt{\omega - \omega_U}}{\omega - \omega_U + \epsilon} \theta(\omega - \omega_U) \quad , \tag{4}$$

where $\theta(\omega)$ is the step function, ω_U is the (upper) BGE, ϵ is the edge-smoothing factor, and K is a suitable constant. A similar dependence (but singular at the BGE) can be derived from the "effective-mass" approximation to the isotropic photon dispersion relation. The dependence (4) was obtained by introducing a nonzero parameter ϵ to the "effectivemass" result with the effect to smooth the singularity of the DOM. The modes below the lower edge are neglected. It is a good approximation if the gap is sufficiently wide. Secondly, I neglect frequency and space dependences of the coupling parameters G_{λ} . The DOM and the coupling parameters are important quantities for determining the vacuum-field response function [12] which for a given DOM $\rho(\omega)$ is $\Gamma(\omega) = 2\pi |G_{\omega}|^2 \rho(\omega)$. (Here the coupling parameters are labeled by ω instead of λ .) The value $\Gamma(\omega_A)$ represents the SPE rate from the atom. However, this rate has its traditional physical meaning only for the SPE to a smooth reservoir. Near a sharp edge of the photonic band gap the atom decays neither exponentially nor completely [13,14,4,5]. In spite of the simplifications described above, the model enables to recover many qualitative aspects of the atom-field dynamics in PBS. It was used, for example, in Refs. [4,15].

For numerical simulations, I also introduce other approximations but these are already approximations to the "ideal" model defined above. Firstly, I discretize the electromagnetic field, i.e., I calculate with a spectrum of discrete (but sufficiently dense) modes. I calculate the frequencies ω_{λ} of the modes from the equation $\int_{0}^{\omega_{\lambda}} \rho(\omega) d\omega = \lambda$ where $\rho(\omega)$ is a given DOM and λ is a positive integer number labeling the modes. Secondly, I introduce a cutoff on the field modes. I have found that the cutoff $\omega_{cut} \approx 3 \omega_U$ is sufficient to obtain cutoff-independent results in a good approximation. Thirdly, I omit vectors $|g, 1_{\omega}, 1_{\omega'}\rangle$ if at least one of the frequencies ω , $\omega' \ (\omega \neq \omega')$ is largely detuned from the atomic transition (i.e., if it lies outside of an interval $[\omega_U; \omega_I]$, where ω_I is a value sufficiently larger than both ω_U and ω_A .) I also omit vectors $|e,2_{\omega}\rangle$ for the modes outside of the interval $[\omega_U;\omega_I]$. The fourth approximation to the ideal model further reduces the number of the modes. It consists of employing a DOM which is decreased [in comparison with the DOM (4)] in less interesting physical regions (far above the BGE) with the simultaneous increase of the corresponding coupling parameters. I have found that the accuracy of the approximations performed to the "ideal" model is quite sufficient. The ap-



FIG. 1. Excited-state population of the stimulately emitting atom and (for comparison) of the spontaneously emitting one. The atomic transition is tuned inside the gap near the BGE ($\omega_A = 0.98\omega_U$). Other important numerical values are $\omega_U = 1$, $C = 0.001\omega_U^{3/2}$, $\epsilon = 0.001\omega_U$, and $\tau_0 = 1500/\omega_U$.

proximations enable to reduce many times the number of the considered degrees of freedom.

I write the Schrödinger equation in the bare-state basis which gives a set of simple first-order differential equations. I use the modified midpoint method (MMPM) [16] to integrate this set of equations.¹ In what follows I present some of the results if the atomic transition frequency $\omega_A = 0.98\omega_U$, i.e., it is inside the gap near the BGE. The initial state of the field is chosen with the parameter $\tau_0 = 1500/\omega_U$.

Figure 1 (solid line) shows the time-dependent probability that the atom which emits stimulately would be detected in its excited level. For comparison it is very useful to plot also the curve (dashed line) corresponding to the case if there were no initial field. (It would be just SPE.) We can see that there is a noticeable difference between the spontaneous and stimulated decay although it was caused by the single initial photon. Both decays are incomplete. This feature arises because the system exhibits the so-called bound state of the atom and (localized) photon [17], i.e., there exists a singleexcitation eigenstate of the Hamiltonian (2) with an eigenenergy within the gap [4]. To show the agreement of the numerical results for the SPE with the exact theory of Kofman *et al.* [4] I plot also these exact result by dots. It assures that the mode distribution is sufficiently dense so that there are

¹For the purpose of numerical calculations I have implemented the MMPM algorithm exactly as it is described in the *Numerical Recipes*, using the single precision. I have separated each probability amplitude into its real and imaginary part. The calculations corresponding to Fig. 1 used 500 time steps and each step was divided into *nstep* = 32 substeps. The norm of the state vector is an important parameter for testing the accuracy of the calculations. The worst value of the norm for the presented result was 0.997 98. The size of the Hilbert subspace was 603 049. The memory consummation was 38 MB. The calculation spent 1564 CPU minutes on the machine with the Pentium 200 processor. I have successfully ran also larger calculations (up to one million vectors of the Hilbert subspace) when I was testing the approximations to the ''ideal'' model.



FIG. 2. (a) Initial photon spectrum, i.e., initial populations of the modes (multiplied by proper factors for convenience) considered for the stimulated emission process. (b) Time-averaged (over the interval [900;1500]/ ω_U) photon spectrum in the stimulated emission process. The plotted quantities correspond to parameters used for Fig. 1.

no recurrences on the time scale shown on the figures. A very little difference between the exact results and the numerical ones is caused by the approximations to the "ideal" model, *not* by numerical errors.

In what follows a term "photon spectrum" is used for the set of expectation values of the photon-number operators of the modes (in a given quantum state of the system) multiplied by the factors $\omega_U \rho^{\text{PBS}}(\omega_\lambda)$. Figure 2(a) shows the photon spectrum for the initial state of the field² which is given by the amplitudes c_λ [see Eq. (3)]. The phase of the oscillations depends on the parameter τ_0 in Eq. (3). Figure 2b represents for the field in the STE process the *time-averaged*

values of the photon spectrum. The averaging is performed over the interval $[900; 1500]/\omega_U$. The purpose of the averaging is to show that the oscillating shape of this photon spectrum is only weakly dependent on the time instant at which it is calculated. This shape is strongly correlated with the shape of the initial spectrum. This behavior is explained as a typical feature of STE: the atom predominantly emits into the initially occupied modes.

The results of this Brief Report have a relation to the results for the resonance fluorescence (RF) published by other authors. In Ref. [9] the authors analyzed RF using a two-level model of an atom with its transition near a BGE. In the simulation the authors included the effects of the laser field as well as the SPE and absorption from single-photon states. They did not include the effects of absorption and STE induced by photons occupying multiphoton states near the BGE. In spite of that, their model should give correct results as the intensity of the laser field is usually much larger than the intensity of the quantum field created in the RF process. For very weak laser fields the effect of the absorption and STE due to the localized photons might have a noticeable influence. Another scheme of the RF in a PBS (using a three-level Λ model) was analyzed in Ref. [8]. In this case the photons emitted on the free-space-like transition propagate away from the atom and does not influence it.

In conclusion, I have presented basic features of the stimulated emission (STE) from a two-level atom in a photonic band structure. I have considered conditions of this process quite different from the conditions used by other authors [4]. I have analyzed the system when the initial multimode field is a superposition of single-photon states with the spectrum of energy localized near the band-gap edge. I assumed that the atomic transition is (quasi)resonant with the band-gap edge. If the excited atom is allowed to interact with the single-photon field the decay of the atom can be significantly influenced by the presence of the initial photon. The wave packet of the light (including also the light emitted by the atom) particularly remains spatially localized around the atom for a long time because of multiple reflections of light on the boundaries of the structure. On the contrary, in free space a wave packet propagates away from its initial region thus having less influence on the atom. The shape of the photon spectrum radiated in the STE is strongly correlated with (similar to) the shape of the initial photon spectrum. It is a manifestation of the STE when the atom predominantly emits into the initially occupied modes. Finally, I expect that the straightforward numerical method used here can be also useful for other problems (e.g., superradiance or study of the emission stimulated by various single- or two-photon wave packets) in which one has to consider a large number of degrees of freedom and other methods are inefficient.

I thank Dr. Drobný and Prof. Bužek for useful discussions and for the reading of the manuscript.

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²Oscillations of this type in the mode populations can really arise in an environment of a photonic crystal. For example, it can be a feature of the light originating from SPE near a BGE as it can be readily explained using the theory in Ref. [4]. Oscillations are not present in the spontaneously emitted photon spectra described in Refs. [14,4] because the authors did not consider the contribution of the so-called localized light arising from the bound state of the atom and the field. The localized light does not propagate away from the structure and so it cannot be detected by devices placed outside of the localization region. However, this light can effect behavior of an atom placed inside this region.

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