Singular behavior of the photon density of states and the self-energy function of an electron in photonic crystal

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Abstract. We show that Van Hove singularities in the behavior of the photon density of states in a photonic crystal results in a singular behavior of the self-energy functions of atomic states that describe the interaction of the atom with vacuum. This is shown to have a significant effect on processes of quantum interference from atoms in the PC medium.

1. Introduction
There has been a growing interest in the study of photonic crystals (PC) which are periodic systems consisting of dielectric materials with different refractive indices. The variation of the photon density of states (DOS) being a result of a modification of electromagnetic field in PCs leads to quantum effects, including the coherent control of the spontaneous emission [1], the appearance of photon-atom bound states [2], the non-Markovian character of radiative decay [3], enhanced quantum interference effects [4] and the localization of superradiance near the photonic band edge [5]. In Ref. [6] it has been shown that a strong modification of the interaction of a charged particle with its own radiation field in photonic crystals results in the fact that in the PC medium the electron mass changes its value. This effect is important not only from the fundamental point of view but also for applications. It opens new ways of using PCs [7] that in contrast to the ordinary ways are not based on the band gap effect. The modification of the self-interaction of electrons affect not only the electron mass but also the character of the interaction of photons with atoms in PC’s. The aim of the present paper is to show that this can have a significant effect on processes of resonance fluorescence from atoms in the PC medium.

2. Resonance fluorescence from atom in PC’s and vacuum modes
The recent experimental observations of the resonance fluorescence from self-assembled quantum dots, being atom-like two-level emitters, have shown [8] not only the asymmetry which for some detuning becomes very significant but also surprising sideband linewidths, while the standard theory predicts that the fluorescence spectrum should consist of a symmetric triplet. This discrepancy between the experiment and the theory could originate from the fact that the ordinary theory of the resonance fluorescence does not take into account the fact that the effect of the vacuum modes on the spectrum of resonance fluorescence may be significant.
In the standard theory it is assumed that in the case when \( \omega_L \) is close to the frequency \( \omega_R = \omega_e - \omega_g \) of the transition between two bound states \(|g\rangle\) and \(|e\rangle\) only the resonance mode is included into the strong atom-laser interaction. However, as it has been shown in Ref. [9], the vacuum modes that manifest themselves in nonradiative transitions between the dressed states can give a significant contribution to this interaction. In quantum optics the strong atom-laser interaction is usually described by using the two-level model and the rotating wave approximation (RWA) [10], and the dressed states are defined as eigenstates of the system Hamiltonian \( H_{RWA} \): 
\[
|\pm, n\rangle = a_\pm |e, n\rangle + b_\pm |g, n\rangle, \quad a_\pm = \cos \theta_n, \quad b_\pm = -\sin \theta_n, \quad \text{where} \quad |e, n\rangle \ (|g, n\rangle) \text{ denotes the state containing the atom in the bare state } |e\rangle \ (|g\rangle) \text{ and } n \text{ photons in the laser mode and } \theta_n \text{ is the mixing angle defined by } \tan(2\theta_n) = -\Omega_n/\Delta \text{ with } \Omega_n \text{ and } \Delta \text{ being the Rabi frequency } \Omega_n = 2g_L\sqrt{n+1} \text{ and detuning respectively. The energies of these states are } E_{\pm, n} = (n + 1/2)\omega_L + (\omega_e - \omega_g)/2 \pm \Omega_R^{(n)}/2 \text{ with } \Omega_R^{(n)} \text{ being the generalized Rabi frequency.} 
\]

The states dressed by the interaction of the atom with the resonance laser field are not dressed by its interaction with the vacuum modes, and in our investigation of the problem we do not assume a priori that this interaction is weak in any case and we use nonperturbative methods of its description based on the the generalized dynamical equation (GDE), which [11] has been derived as a direct consequence of the first principles of quantum physics. Being equivalent to the Schrödinger equation in the case when the interaction in a quantum system is instantaneous, GDE allows one to extend quantum dynamics to the case of nonlocal-in-time interactions. This equation has been proven to be a useful tool for solving various problems in nuclear physics [12, 13], atomic physics [7, 14–17] and quantum optics [9, 18]. Within this approach the QED bound state problem is solved by using the formalism of the self-energy function \( C_n(z) \) (see for details Ref. [19]), that describes the interaction of the particles in the state \(|n\rangle\) with the vacuum. The self-energy QED corrections to the energies \( E_n^{(0)} \) of the bare states are determined by the equation \( z - E_n^{(0)} - C_n(z) = 0 \) where \( C_n(z) \) in turn are determined by GDE. In the first approximation the solution of this equation is 
\[
E_n \equiv E_n^{(0)} + C_n^{(0)}(E_n^{(0)}) \equiv E_n^{(0)} + \Delta E_n^L - 4\Gamma_n, 
\]

where \( E_n \) is the energy of the real dressed state, \( E_n^L \) is the Lamb shift, \( \Gamma_n \) is the natural level width, and \( C_n^{(0)}(z) \) is determined by the equation 
\[
dC_n^{(0)}(z)/dz = -\langle n|H_I\Sigma_G^{(0)}(z)H_I|n\rangle, 
\]

with \( H_I \) being the QED Hamiltonian. For this approximation to be valid, probability amplitudes of the nonradiative transitions between the states with the same total angular momentum \( J \), its projection \( J_z \) and parity must be much smaller than the energy distance between these states. In addition the variation of the function \( C_n(z) \) with the energy must be negligible on the energy interval of order of the value of the Lamb shift. This takes place in the case when the atom is in free space. In fact, in this case the energy distance between the states with the same \( J, J_z \) and parity are of order of \( \alpha^2 m_e \), while the probability amplitudes of nonradiative transitions between them are of order of \( \alpha^3 m_e \), and the self-energy function varies significantly with the energy only on energy intervals of order \( m_e \). The situation is dramatically changed in the case of an emitter subject to resonance laser field because the energy distance between dressed states \(|+, n\rangle\) and \(|-, n\rangle\) having the same \( J, J_z \) and parity equals to the Rabi frequency. As a result the nonradiative transitions between these states begin to play an important role. At leading order the probability amplitudes \( \langle \pm, n|\Sigma(z)|\mp, n\rangle \) of these transitions are given by the formula [9] 
\[
\langle \pm, n|\Sigma(z)|\mp, n\rangle = \cos \theta \sin \theta (C_{g}^{(0)}(z) - C_{e}^{(0)}(z)), \quad \text{where} \quad C_{g}^{(0)}(z) \text{ and } C_{e}^{(0)}(z) \text{ are the self-energy functions of the bare states } |g\rangle \text{ and } |e\rangle \text{ respectively. At the same time, in the case of an atom being in free space the energy interval of order } \Omega_R \text{ is too small for the variation with energy of } \langle \pm, n|\Sigma(z)|\mp, n\rangle \text{ to be noticeable. In this case the energy dependence of } \langle \pm, n|\Sigma(z)|\mp, n\rangle \text{ can be neglected, and they can be regarded as matrix elements of an additional term in the Hamiltonian describing the interaction of the atom with resonance laser field. Adding such a term to the RWA Hamiltonian will lead only to a change in the mixing angle } \theta_n, \text{ and, as a consequence, will not give rise to asymmetry of the Mollow spectrum. However, as we show below, because}
of the singular behavior of the photon density of states the variation of self-energy functions \( C_p(z) \) and \( C_e(z) \) of an atom in the PC medium on an energy interval compared to the energy difference between the dressed states \(|+, n\rangle\) and \(|-, n\rangle\) can be very significant, and hence the vacuum modes are involved into the strong atom-laser interaction.

### 3. Self-energy functions of an electron in PC

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Using Eq. (2) and (3) we get

\[
C_p^e(z) = -\frac{\alpha E_K}{m_e \pi^2} \sum_n \int_{FBZ} d^3 k \frac{\sum_{G, \lambda} \left| \epsilon_{Gn}^{G1} \right| \left| \epsilon_{Gn}^{G2} \right| \left| \epsilon_{Gn}^{G3} \right|}{\omega_{kn}} z - E_K - \omega_{kn},
\]

where \( E_K = \frac{p^2}{2m_e} \) and \( (\epsilon_{G\lambda})_p \) are the projections of the polarization vectors onto the axis of the electron momentum. In order to eliminate these, we can assume that summing over \( G \) and \( \lambda \) averages these values, yielding a factor of 1/2. Further estimates can be made with unknown solutions to Maxwell equations in a PC medium by building a model analogous to the one described in [6]. In this model Eq. (4) takes form

\[
C_p^e(z) = -\frac{\alpha E_K}{m_e \pi^2} \frac{\Lambda}{2 \pi} \int_0^\Lambda \frac{d\omega}{\omega} \frac{N_p(\omega)}{z - E_K - \omega},
\]

where \( N_p(\omega) = N_{DOS}(\omega) D(\omega), N_{DOS}(\omega) \) is the photon density of states \( N_{DOS}(\omega) = \frac{1}{4\pi} \sum_{n} \int_{FBZ} d^3 k \delta(\omega - \omega_{kn}) \) and \( D(\omega) = \frac{1}{2} \sum_{G, \lambda} \left| \epsilon_{Gn}^{G1} \right|^2 \left| \epsilon_{Gn}^{G2} \right|^2 \left| \epsilon_{Gn}^{G3} \right|^2 \). Here the cutoff \( \Lambda \) is imposed to separate the momentum region relevant for the variation of \( C(z) \) at low energies. Real density of states and, as a consequence, \( N_p(\omega) \) have very complicate behavior because of Van Hove singularities [20], see Fig 1(a). In the case when pole of the integrand in (4) is in the vicinity of this singularities, the value of the \( C(z) \) can be very significant. To demonstrate this let us consider the influence of some critical points on the \( C(z) \). For this we determine \( N_p(\omega) \) so that it contains the same critical points as the real density of states.

As it follows from the results of calculations, the variation of the electron self-energy functions and as a consequence, the variation of the atomic self-energy functions \(|g\rangle\) and \(|e\rangle\) are very significant, and, as it follows from the comparisons of the results presented on Fig. 1(a) and Fig. 1(b) the singular behavior of the self-energy functions is a consequence of Van Hove singularities.
Figure 1. a) Density of states of the 2D PC composed of a hexagonal lattice of dielectric cylinders with permittivity $\epsilon = 12$ and radius $a/d = 0.2$ where $d$ is period of PC. b) The self-energy function $C_p^e(z)$ of a free electron with $E_K = 3$ eV placed in PC medium calculated using Eq.(4)

4. Conclusion
We have shown that Van Hove singularities in the behavior of the photon density of states results in a singular behavior of the self-energy functions of the atomic states $|g\rangle$ and $|e\rangle$. This means that under certain conditions the vacuum modes are involved into the strong atom-laser interaction. Moreover, coming these modes into play can make this interaction much more stronger, and this can have a significant effect on processes of resonance fluorescence from atoms in the PC medium.

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