Modification of the interaction of an electron with its own radiation field in photonic crystals with high-refractive layers

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Abstract. The self-energy interaction of atoms placed in air voids of one-dimensional photonic crystals with high-refractive layers is considered. Modification of the interaction of an electron with its own radiation field in the photonic crystal medium gives rise to a correction to its mass and kinetic energy. We demonstrate the photonic density of states of the periodic structure and the dependence of the mass correction of the valence electron of hydrogen atom and the alkali metals on the refractive index of the one-dimensional photonic crystal based on alternating amorphous hydrogenated layers of silicon nitride a-SiNx:H and vacuum, and layers of the high refractive index metamaterial consisting of Au nanoparticles with a dielectric matrix based on HfO2 and vacuum. The tunability of these materials gives rise to the tunability of the mass correction over a wide range. It is shown that the effect under study leads to significant shifts in the energy levels of atoms which is important for controlling physical and chemical processes, creating new linear light sources, and He-Ne-like lasers.

1. Introduction
Photonic crystals (PCs) made from two or more dielectrics with different refractive indices periodically arranged in spatial directions have great attention in photonics and quantum technologies due to the ability of control in the broad spectral range the optical properties such dispersion relations, the width of the photonic bandgap, optical density of states, etc. [1,2]. PCs are the promising media for observing and studying quantum electrodynamic (QED) effects such as the control of spontaneous emission of atoms, quantum dots and qubits placed in the periodical structure of PCs [3, 4], amplification of quantum interference and creation of dark states [5], control of the electron mass [6,7].

In [6] the effect has been predicted that a strong modification of the electromagnetic interaction of an electron with its own radiation field in air voids of the PC medium gives rise to the modification of an electromagnetic mass of a charged particle. According to the Kramers principle, the physically observed mass of the electron $m_e$ is represented as the sum of the mechanical mass $m_0$ and the electromagnetic mass $m_{em}$ which is formed due to the interaction of an electron with its own radiation field [8]. The electromagnetic mass $m_{em}$ cannot
be calculated because of the non-renormalizable ultraviolet divergences [9]. Modification of the electromagnetic interaction in the PC medium leads to the correction $\delta m_{pc}$ of an electromagnetic mass $m_{em}$ which is not observable in free space. This correction $\delta m_{pc}$ is a finite, and can be calculated. An important property of the self-energy correction $\delta m_{pc}$ is the dependence on the electron momentum in PCs that gives rise to the significant shifts of the energy levels of atoms placed in air voids of the periodical structure of PCs. Under certain conditions these shifts can be comparable to the energy of the ordinary atomic transitions.

In this paper, we calculate the correction to the mass of an atomic electron placed in air void of one-dimensional PC because this periodical structure is interesting of the theoretical and practical point of view. We consider one-dimensional PCs consisting of alternating amorphous hydrogenated layers of silicon nitride (a-SiN$_x$:H) [10] and vacuum, as well as layers of the high refractive index metamaterial consisting of Au nanoparticles with a dielectric matrix based on HfO$_2$ [11–13] and vacuum. We show the dependence of the correction to the atomic electron mass on the refractive index of the PC medium. To evaluate the interaction of an electron with its own radiation field using Coulomb gauge, the calculation of electromagnetic fields in a dielectric periodic structure is carried out by numerically solving of the Maxwell equations and finding the eigenfunctions (distribution of the magnetic and electric components of the field) and eigenvalues (dispersion relations). The electromagnetic field was calculated using the Plane Wave Expansion Method (PWE) [1], and the dispersion relations were calculated using the Transfer-Matrix Method (TMM) [14]. The calculation of the density of photonic states (DOS) in one-dimensional PCs is described in [15] in detail. We present the calculated DOS for the above two types of one-dimensional PCs.

2. The correction to the electromagnetic mass of an electron in the PC medium

Interaction of an electron with its own radiation field in vacuum leads to the correction its physical mass $m_e$ known as an electromagnetic mass $m_{em}$ that is included into the physical mass $m_e$. The electromagnetic mass is an infinite quantity due to the non-renormalizable ultraviolet divergences. However, in the periodical boundary conditions of the PC medium the photons have a Bloch structure, and the electromagnetic mass of an electron in the PC medium will differ from the case of vacuum. The corresponding diagrams are shown in figure 1 (a, b). Thus, modification of the electromagnetic vacuum in PCs leads to the change in $m_{em}$ by the value of the difference in the electromagnetic mass – the correction $\delta m_{pc}$ which is the finite, therefore, observable. It is important that the self-energy interaction of the free electron is the first term

![Figure 1](image)

**Figure 1.** The self-interaction diagram of an electron with (a) virtual photons in vacuum and (b) photon Bloch modes of the PC medium

in the expansion of the scattering amplitude. The second term which is smaller in order is the interaction of an electron with itself and with the atomic nucleus using virtual photons. This second-order contribution is known as the Lamb shift [8].
In [6] it has been shown that the correction to the electron mass propagating with
momentum $\mathbf{p}$ in a void of the PC medium is an anisotropic observable and is described by an operator (here
and below, we use the natural system of units in which $\hbar = c = 1$):

$$\delta m_{pc}(\hat{\mathbf{I}}_p) = \frac{\alpha}{\pi^2} \left[ \sum_n \int_{FBZ} d^3k \, \frac{1}{\omega_{kn}} \sum_G \left| \hat{\mathbf{I}}_p \cdot \mathbf{E}_{kn}(G) \right|^2 - \int d^3k \, \frac{2}{2k^2} \sum_{\lambda=1}^2 \left| \hat{\mathbf{I}}_p \cdot \varepsilon_\lambda(k) \right|^2 \right]$$

(1)

with $\hat{\mathbf{I}}_p = \frac{\hat{\mathbf{p}}}{|\hat{\mathbf{p}}|}$ being an operator of the direction of the electron momentum, $\varepsilon_\lambda(k)$ is the unit
vector of the field polarization ($\lambda$) in free space, $n$ is a band index, the value of $k$ is limited
by the first Brillouin zone (FBZ) [14], $G$ is the reciprocal lattice vector of the photonic crystal
and $\alpha$ is the fine-structure constant. $E_{kn}(G)$ are the coefficients in the plane-wave expansion
$E_{kn}(r) = \sum_G E_{kn}(G)e^{i(k+G) \cdot r}$ of the Bloch eigenfunctions $E_{kn}(r)$. The polarization structure
of the electromagnetic field in one-dimensional PC is described as:

$$E_{kn}(G) = \sum_{\lambda=1}^2 E_{kn\lambda}(G)\varepsilon_\lambda(k_G),$$

(2)

where $\varepsilon_1(k_G)$ and $\varepsilon_2(k_G)$ are unit vectors of the TE (transverse-electric) and TM (transverse-
magnetic) polarization, correspondingly, $k_G = k + Ge_z$ (see figure 2). Thus, for one-dimensional

Figure 2. The polarization structure of the electromagnetic field in one-dimensional PC

PC the operator of the self-energy correction equation (1) can be rewritten as [16]

$$\delta m_{pc}(\hat{\mathbf{I}}_p) = A + \left( \hat{\mathbf{I}}_p \cdot \hat{\mathbf{I}}_{pc} \right)^2 B,$$

(3)

where $\hat{\mathbf{I}}_{pc}$ is the unit vector of the one-dimensional PC crystal axis that coincides with vector $e_z$ and

$$A = \frac{\alpha}{\pi} \sum_n \int d\rho \, d\mathbf{p} \int_{FBZ} dk_z \left( \frac{|E_{kn1}(G)|^2}{\omega_{kn1}^2} \frac{k^2_p}{k^2_p + k^2_G z} + \frac{|E_{kn2}(G)|^2}{\omega_{kn2}^2} \right) - \frac{4\alpha}{3\pi} \int d\mathbf{k},$$

$$B = \frac{\alpha}{\pi} \sum_n \int d\rho \, d\mathbf{p} \int_{FBZ} dk_z \left( \frac{|E_{kn1}(G)|^2}{\omega_{kn1}^2} \frac{2k^2_p - k^2_G z}{k^2_p + k^2_G z} - \frac{|E_{kn2}(G)|^2}{\omega_{kn2}^2} \right).$$
Here $\omega_{kn1}$ and $\omega_{kn2}$ are dispersion relations for TE and TM Bloch modes satisfying transcendental equation [14]. The coefficients $A$ and $B$ can be calculated numerically using the PWE and TMM methods. These coefficients take into account the contribution from the polarization structure of the electromagnetic field $E_{kn\lambda}(G)$ and the corresponding dispersion relations $\omega_{kn\lambda}$ in the one-dimensional PC medium. The self-energy correction to the atomic electron mass is calculated by using matrix elements $\langle \Psi | \delta m_{pe} (\hat{I}_p) | \Psi \rangle$ with the corresponding states of an charged particle.

3. The spectral dependencies of the high-refractive layers of the periodical structure and photonic DOS of one-dimensional PC

Photonic DOS is an important property of the micro- and nanostructures. DOS characterizes the number of allowable eigenstates of the electromagnetic field in a certain photon energy range in the PC medium. Calculation of DOS has been carried out on the base of the following equation [15]:

$$N^{1D}_{DOS}(\omega) = \rho_\lambda'(\omega) = \left[ V / (2\pi)^2 \right] 2 \sum_n \int_0^{\sqrt{T_\lambda\omega/c}} \beta d\beta / \left( \partial \omega / \partial k_B^p \right),$$

(4)

where the integration is performed in the inverse, phase space using the photon wave vector $k = (k_B, \beta \cos \varphi, \beta \sin \varphi)$ and the tangential wave number $\beta = \sqrt{k_y^2 + k_z^2}$. During the integration, the eigenstates of the electromagnetic field with the same frequencies are summed within the FBZ, and the subsequent summation by band index $n$ is performed over all zones.

Recently a great progress has been achieved in the design of metamaterials with unnaturally highly tunable refractive indices [11–13]. We can significantly enhance the effective refractive index of these materials by control the geometrical parameters such as the size $(a)$ of the metal nanoparticles of metamaterials and distance-gap $(g)$ between them. We consider one-dimensional PCs consisting of alternating amorphous hydrogenated layers of silicon nitride (a-SiN$_x$:H) $(n_h (eff) = 3)$ [10] and vacuum, as well as layers of the high refractive index metamaterial $(n_h (eff) = 15)$ consisting of Au nanoparticles $(a = 30 \text{ nm}, g = 0.7 \text{ nm})$ with a dielectric matrix based on HfO$_2$ [11–13] and vacuum. The spectral dependencies of the high-refractive layers of the periodical structure are shown in figure 3 (a, b). In this paper, we consider only the real part of the refractive indices of the above-mentioned materials. We use the step function of the effective refractive index $n_h (eff) = 3$ until the maximum photon energy $\omega_{kn1}^{\text{max}} = 6.4 \text{ eV}$ and $n_h (eff) = 15$ until the maximum photon energy $\omega_{kn2}^{\text{max}} = 10.65 \text{ eV}$ for figure 3 (a) and figure 3 (b), correspondingly.

Figure 4 (a, b) shows the corresponding DOS for two types of one-dimensional PCs consisting of layers a-SiN$_x$:H and metamaterials (figure 3 (a, b)) as the high-refractive layers and intermediate vacuum layers. The periodic structure of the PC medium significantly influences on the electromagnetic field in comparison with the case of vacuum. Sharp peaks (Van Hove singularities [17]) occur in DOS that corresponds to the edges of the photonic bandgap in the dispersion relations of PCs, and indicate a large number of eigenstates of the electromagnetic field and the tendency of some components of the group velocity of photons to zero (denominator of equation (4)). Accordingly, DOS is significantly modified with an increase of the PC refractive index which leads to a significant modification of the self-interaction of an electron with its own radiation field.

It is important that the self-energy correction $\langle l, ml | \delta m_{pe} (\hat{I}_p) | l, ml \rangle$ depends only the orbital quantum number $l$ and its projection $m_l$ of the atomic electron state functions. Thus, we estimate the value of the self-energy corrections $\langle \delta m_{pe} \rangle$ to the electromagnetic mass of the valence electron in the s-state $(l = 0, m_l = 0)$ of hydrogen atom and the alkali metals placed in air voids of one-dimensional PC by performing an exact calculation of the electromagnetic fields in two types
Figure 3. The spectral dependence (a) for layers of a-SiN$_{x}$:H, (b) for metamaterial consisting of AuNPs ensemble ($a = 30$ nm, $g = 0.7$ nm) coated with HfO$_2$ (thick blue solid line) extracted from the experiment ($n_d(\omega) \approx \sqrt{\varepsilon_d(\omega)}$ of the HfO$_2$) (red dashed line) [12]. This curve for the same region of frequencies as the experimental one has been plotted using equation $n_{h\text{eff}}(\omega) = [(a/g)\varepsilon_d(\omega)]^{1/2}$ [11]. The rest part of this curve has been chosen to provide the fact that at the high frequencies $n_{\text{eff}} \to 1$ (green dash-dotted line). The average refractive indexes (a) $n_{h\text{eff}} = 3$ and (b) $n_{h\text{eff}} = 15$ are given for the first and second material at maximum frequency $\omega_{kn}^{\text{max}} = 6.4$ eV and $\omega_{kn}^{\text{max}} = 10.65$ eV, respectively.

Figure 4. Photonic DOS for one-dimensional PCs with the high-refractive layers (a) a-SiN$_{x}$:H with $n_{h\text{eff}} = 3$ and (b) metamaterials consisting of Au nanoparticles with a dielectric matrix based on HfO$_2$ with $n_{h\text{eff}} = 15$. In both cases, the relative layer thickness $d_{h}/T = 2/3$. As the other medium, a vacuum layer with a relative thickness $d_{l}/T = 1/3$ was taken. The dashed curve corresponds to DOS of unpolarized light modes in vacuum. The period $T$ of one-dimensional PC is 750 nm.

Figure 5 shows the dependence of the self-energy correction $\langle \delta m_{\text{pc}} \rangle$ on the refractive index $n_{h}$ of one-dimensional PC. This correction quadratically increases with growing $n_{h}$ because DOS
Figure 5. The dependence of the self-energy correction $\langle \delta m_{pc} \rangle$ on the refractive index $n_h$ of one-dimensional PC. One-dimensional PC has the following parameters: $d_l/T = 1/3$, $\max(n_h) = n_{h\,(\text{eff})} = 15$ ($\omega_{\text{max}} = 10.65$ eV) and $d_h/T = 2/3$. The period $T$ of one-dimensional PC is 750 nm.

significantly modifies under this condition.

4. Conclusion

In conclusion, modification of the electromagnetic field in the PC medium leads to modification of the interaction of an electron with its own radiation field that is expressed as the self-energy correction to the electromagnetic mass of a charged particle. This correction is an anisotropic observable depending on the electron momentum. The self-energy correction quadratically increases with growing the refractive index $n_h$ of the PC medium. The use of new artificial optical media like metamaterials with the tunable refractive index of the PC layers allows us to control the value of the self-energy correction, and therefore to shift the energy levels of atoms in a controlled manner. We believe that the effect under study can be used to precisely adjust the energy levels of atoms, control physical and chemical processes, and can bring us several steps closer to creating a new type of linear sources based on PCs which are important for photonics and quantum technologies.

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