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Self-energy shift of the energy levels of atomic hydrogen in photonic crystal medium

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Abstract. Corrections to the average kinetic energy of atomic electrons caused by the change in electron mass in the photonic crystal medium are investigated. Corresponding shift of energy levels of atoms placed in a photonic crystal is shown to be of order of the ordinary Lamb shift.

The investigation of photonic crystals (PC) is an actual problem today. The main feature of such media is the periodic modulation of dielectric constant along one, two or three directions of space. It yields to the range of forbidden frequencies in a material called photonic band-gaps (PBG). Unusual optical properties of the PC medium stimulate a wide range of its practical applications [1]. Another interesting field of study is quantum electrodynamics (QED) in PC medium. It has been shown that modification of photon density of states (DOS) in PC's lead to the strong emitter-photon coupling [2–4], coherent control of spontaneous emission [5–7], appearance of photon-atom bound states [2, 8, 9] etc. Special attention was given to the modification of the Lamb shift [2, 8, 10–14] in atoms placed in the photonic crystal medium. By definition the Lamb shift in atoms is caused by the QED corrections to the Coulumb interaction between electrons and the atomic nucleus (see figure 1a) that gives the leading order contribution to the energy of atomic states. This interaction is modified by the processes in which the virtual photons come into play (see figure 1b). The contribution to atomic energy levels from these processes is just the Lamb shift. In principle one should account for the processes of the self interaction of the atomic electrons shown in figure 1c. In the case of atoms in free space these processes contribute only to the electron mass and are subtracted by the counter-terms of the renormalization. However, as it has been shown in Ref. [15], a modification of the of the interaction of the electron with its own radiation field in a PC gives rise to the fact that contributions from the processes in a PC shown in figure 1c differ profoundly from those in free space, and, as a result, these self-energy processes can play an important role. First of all, they change the mass of an electron in the PC medium [15]. In addition they contribute to the kinetic energy of atomic electrons in the PC. The aim of this paper is to investigate this correction to the energy levels of atoms in the PC medium.

The change of the value of the kinetic energy of an electron δE is the difference between its values in the PC medium and in vacuum:

$$\delta E^{pc} = E^{pc} - E^{vac}.$$

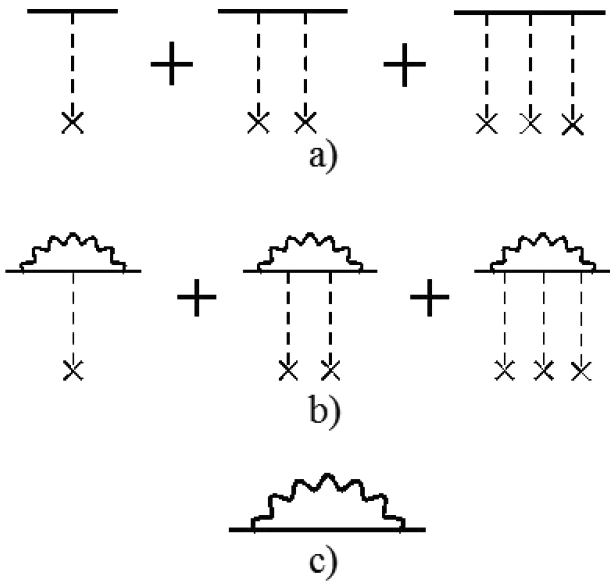

Figure 1. a) Processes of the Coulumb interaction between the nucleus and atomic electrons that give the leading order contribution to the energy of atomic states. b) Processes in which between emission and reabsorbtion of a photon a bound electron interacts with the Coulumb field of the nucleus. Just these processes give rise to the Lamb shift. c) Process in which an atomic electron emits and reabsorbs a photon virtually without any interaction with the nucleus. This process changes the electron mass $m_e \to m_e + \delta m_e$ and the kinetic energy $\frac{\mathbf{p}^2}{2m_e} \to \frac{\mathbf{p}^2}{2m_e} - \frac{\mathbf{p}^2}{2m_e}\frac{\delta m_e}{m_e}$.

The one-loop low-energy contribution to the kinetic energy of an electron propagating with momentum $\mathbf{p}$ in the PC medium and in the free space in the Coulomb gauge takes the form (here and below, we use the natural system of units in which $\hbar = c = \varepsilon_0 = 1$)

$$E^{pc} = \sum_{\mathbf{p}'} \sum_{\mathbf{k}n} \frac{\langle \mathbf{p}| H_I^{pc} |\mathbf{p}'; \mathbf{k}, n\rangle \langle \mathbf{p}'; \mathbf{k}, n| H_I^{pc} |\mathbf{p}\rangle}{\frac{\mathbf{p}^2}{2m_e} - \frac{\mathbf{p}'^2}{2m_e} - \omega_{\mathbf{k}n}}$$

and

$$E^{vac} = \sum_{\mathbf{p}'} \sum_{\mathbf{k}\varepsilon_\lambda} \frac{\langle \mathbf{p}| H_I |\mathbf{p}'; \mathbf{k}, \varepsilon_\lambda\rangle \langle \mathbf{p}'; \mathbf{k}, \varepsilon_\lambda| H_I |\mathbf{p}\rangle}{\frac{\mathbf{p}^2}{2m_e} - \frac{\mathbf{p}'^2}{2m_e} - |\mathbf{k}|}$$

correspondingly, where

$$\langle \mathbf{p}'; \mathbf{k}, n| H_I^{pc} |\mathbf{p}\rangle = -\frac{e}{m_e}\frac{1}{\sqrt{V\omega_{\mathbf{k}n}}} \sum_{\mathbf{G}} \mathbf{p} \cdot \mathbf{E}^*_{\mathbf{k}n}(\mathbf{G}) \delta_{\mathbf{p},\mathbf{p}'+\mathbf{k}+\mathbf{G}}$$

and

$$\langle \mathbf{p}| H_I^{pc} |\mathbf{p}'; \mathbf{k}, n\rangle = -\frac{e}{m_e}\frac{1}{\sqrt{V\omega_{\mathbf{k}n}}} \sum_{\mathbf{G}} \mathbf{p} \cdot \mathbf{E}_{\mathbf{k}n}(\mathbf{G}) \delta_{\mathbf{p},\mathbf{p}'+\mathbf{k}+\mathbf{G}},$$

with $\mathbf{E}_{\mathbf{k}n}(\mathbf{G})$ being the coefficients in the plane-wave expansion $\mathbf{E}_{\mathbf{k}n}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{E}_{\mathbf{k}n}(\mathbf{G}) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$ of the Bloch eigenfunctions $\mathbf{E}_{\mathbf{k}n}(\mathbf{r})$ and having the polarization structure $\mathbf{E}_{\mathbf{k}n}(\mathbf{G}) = e^{\mathbf{G}1}_{\mathbf{k}n}\varepsilon_{\mathbf{G}1} + e^{\mathbf{G}2}_{\mathbf{k}n}\varepsilon_{\mathbf{G}2} + e^{\mathbf{G}3}_{\mathbf{k}n}\varepsilon_{\mathbf{G}3}$. Here $\mathbf{G}$ is the reciprocal lattice vector of the photonic crystal ($\mathbf{G} = N_1\mathbf{b}_1 + N_2\mathbf{b}_2 + N_3\mathbf{b}_3$, where $\mathbf{b}_i$ are primitive basis vectors of the reciprocal lattice) [16]. Thus,

the PC medium correction to the kinetic energy of a free electron is determined by the expression

$$\delta E^{pc} = -\frac{\alpha}{2m_e^2\pi^2}\left[\sum_n \int\limits_{FBZ} \frac{d^3k}{\omega_{\mathbf{k}n}^2} \sum_{\mathbf{G},\lambda} \left|e_{\mathbf{k}n}^{\mathbf{G}\lambda}\right|^2 |\mathbf{p}\cdot\varepsilon_{\mathbf{G}\lambda}|^2 - \int \frac{d^3k}{2\mathbf{k}^2} \sum_{\lambda=1}^{2} |\mathbf{p}\cdot\varepsilon_\lambda(\mathbf{k})|^2\right].$$

If an electron is in the state $|\Psi_n\rangle$, the correction to its energy is given by

$$\delta E_n^{pc} = \langle\Psi_n|\,\delta E^{pc}\,|\Psi_n\rangle\,. \tag{1}$$

Let us consider the example of atomic hydrogen. In this case energy shift (1) takes the form

$$\delta E_a^{pc} = \int d^3p \Psi_a^*(\mathbf{p}) \delta E^{pc}(\mathbf{p}/\,|\mathbf{p}|)\Psi_a(\mathbf{p}), \tag{2}$$

where $|a\rangle = |njlm\rangle$. Assuming that the modification of the interaction of an electron with its own radiation field in PC medium has not a significant effect on the wave function, the electron wave function can be represented in the form $\Psi_{njlm}(\mathbf{p}) = \frac{1}{p}G_{nl}(p)Y_{lm}(\Omega)$, where $G_{nl}(p)$ is the radial function and $Y_{lm}(\Omega)$ is the spherical function. Taking this into account, (2) can be rewritten

$$\delta E_a^{pc} = -\frac{\alpha\,\langle p^2\rangle_a}{2m_e^2\pi^2}\left[\sum_n \int\limits_{FBZ} \frac{d^3k}{\omega_{\mathbf{k}n}^2} \sum_{\mathbf{G},\lambda} \left|e_{\mathbf{k}n}^{\mathbf{G}\lambda}\right|^2 \int d\Omega Y_{lm}^*(\Omega) \left|\frac{\mathbf{p}}{p}\cdot\varepsilon_{\mathbf{G}\lambda}\right|^2 Y_{lm}(\Omega) - \frac{4\pi}{3}\int\limits_0^\infty dk\right], \tag{3}$$

where

$$\left\langle p^2\right\rangle_a = \int\limits_0^\infty dp p^2 G_{lm}^*(p) G_{lm}(p).$$

Thus, equation (3) allows us to calculate the self-energy shift of the energy levels of atomic hydrogen if we know the coefficients in the plane-wave expansion of the Bloch eigenfunctions $\mathbf{E}_{\mathbf{k}n}(\mathbf{r})$. Let us derive the value of this shift for the ground state $|1s\rangle$. The corresponding momentum wave function is

$$\Psi_{1s}(\mathbf{p}) = \tfrac{1}{p}\sqrt{\frac{2}{\pi\beta^3}}\frac{4p}{\left(1+\left(\frac{p}{\beta}\right)^2\right)^2}\frac{1}{\sqrt{4\pi}},$$

where $\beta = m_e\alpha$ and α is fine structure constant. In this case we can simply integrate in (3) over the solid angles Ω for each $\mathbf{G}$ and λ and it yields

$$\delta E_{1s}^{pc} = -\frac{\alpha^2}{2}\frac{4\alpha}{3\pi}\left[\frac{1}{4\pi}\sum_n \int\limits_{FBZ} \frac{d^3k}{\omega_{\mathbf{k}n}^2} \sum_{\mathbf{G},\lambda} \left|e_{\mathbf{k}n}^{\mathbf{G}\lambda}\right|^2 - \int\limits_0^\infty d\omega\right].$$

Taking this into account we can derive the correction to the atomic states in the same way as it was made in Ref. [15]

$$\delta E_{1s}^{pc} = -\frac{\alpha^2}{2}\frac{4\alpha}{3\pi}\int\limits_0^\infty d\omega \frac{N(\omega)-\omega^2}{\omega^2}, \tag{4}$$

where $N(\omega) = N_{DOS}(\omega)D(\omega)$, $N_{DOS}(\omega)$ is the photon density of states

$$N_{DOS}(\omega) = \frac{1}{4\pi}\sum_n \int\limits_{FBZ} d^3k\delta(\omega-\omega_{\mathbf{k}n})$$

and

$$D(\omega) = \sum_{\mathbf{G}} |\mathbf{E}_{\mathbf{k}n}(\mathbf{G})|^2_{|\omega_{\mathbf{k}n}=\omega}.$$

Thus, the function $N(\omega)$ is closely associated with the DOS. The DOS in the PC medium differs significantly from that in vacuum and could demonstrate singular behavior, see, for example, figure 2. The basic features of the PC medium such as photonic band gap and optical density

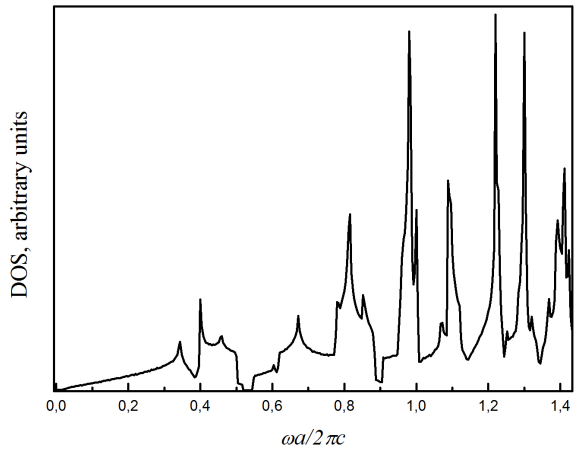

Figure 2. Two-dimensional DOS for a triangular lattice of inversion rods in material with $\epsilon = 12$. The radius of an air cylinder is half of the period of the lattice a.

could be recaptured by the following model function

$$N(\omega) = \omega^2 n_{eff}^3 \left[1 - h \exp\left(-\frac{(\omega-\omega_0)^2}{\sigma^2}\right)\right] F(\omega), \tag{5}$$

where the factor $F(\omega) = n_{eff}^{-3} + (1 - n_{eff}^{-3})/(\exp\{(\omega-\mu)/\tau\} + 1)$ with $n_{eff} \equiv \sqrt{\bar{\varepsilon}}$ and $\bar{\varepsilon}$ being average dielectric constant. Function $F(\omega)$ allows one to take into account that at high enough photon energies $N(\omega)$ must approach the free space DOS. With this model for the parameters $n_{eff} = 3$, $\mu = 15$ eV, $\tau = 0.01$ eV, $\omega_0 = 1$ eV, $h_0 = 0.96$ and $\sigma_0 = 0.07$ eV our calculations of the self-energy shift of the $1s$ level of atomic hydrogen have given $\delta E_{1s}^{pc} = -2.2 \cdot 10^{-5}$ eV that is of order of the Lamb shift of $1s$-state in vacuum. It can be shown that self-energy correction (3) decreases with n as $1/n^2$. As a consequence, the energy levels of Rydberg atomic states should crucially depend on the shifts caused by the change in electrons kinetic energy. This allows one to drive different resonant processes, that could be very important for the optical properties of Rydberg atoms [17].

In conclusion, we have investigated the corrections to the average kinetic energy of atomic electrons caused by the change in electron mass in the photonc crystal medium. These corrections are shown to decrease with n as $1/n^2$ whereas the Lamb shift decreases as $1/n^3$. This fact means that at large values of n the shift caused by the change in electron mass is the main contribution to the correction to energies of atomic states.

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