Islamic Azad University

The Quarterly Journal of
Optoelectronical Nanostructures

Spring 2016 / Vol. 1, No.1

Numerical Calculation of Resonant Frequencies and Modes of a Three-Atom Photonic Molecule and a Photonic Crystal in an External Cavity

Masoud Rezvani Jalal[*1], Fahime Fuladvand[1], Mahshid Habibi[1], Saba Fathollahi[1]

[1]Department of Physics, Malayer University, Malayer.

Abstract: In the present paper, resonant frequencies and modes of a three-atom photonic molecule and a photonic crystal placed within a cavity are numerically calculated. First, governing formulation in transverse electric field mode (TE) is obtained using Maxwell equations. Then, an algorithm based on a finite difference scheme and matrix algebra is presented. The algorithm is then implemented in a computer code developed by the authors. In the first run, resonant modes and frequencies of a linear three-atom molecule in the cavity are calculated. Calculations show that by increasing molecule length,the frequencies first come closer to each other but further increase reverses the process.Such a behavior is related to external cavity walls. In the case of photonic crystal in cavity, calculations show that the field distributions in the ground and first excited states are similar to the case where the cavity is homogeneously filled. On the other hand, calculations show that increasing the optical constant of the crystal decreases the frequencies. Such phenomenon is justified by the fact that light speed is slow in medium of high optical constants.

Keywords: resonant frequencies, resonant mode, TE mode, photonic molecule, photonic crystal.

1. Introduction

Development of nano technology has provided possibility of preparing optical resonators in dimension of micro and nano that are well known as photonic micro cavities [1]. Some examples of these micro cavities are quantum dots, nano plasmonic materials, nano photonic crystal cavities [2], etc. These micro

[*]**Corresponding author: rezvanijalal@malayeru.ac.ir**

cavities are constructed in the form of toroid, sphere, ring, and disk [3-5]. Because of structural similarities between photonic energy levels of a photonic micro cavity and electronic levels of an atom, usually an optical micro cavity is called as a photonic atom. Similarly, a series of several coupled photonic atoms is denominated as a photonic molecule. Many variousforms of photonic molecules from different materials such as silica, semiconductor, and polymer, are visible in the references [3]. Designing and simulation of photonic clusters, grand photonic molecules, and even photonic materials that are made of several photonic atoms is in progress. For example we can hint at photonic chains that are createdby aligning several photonic atoms with very attractive optical and waveguide properties. Photonic meta-materials with wonderful optical properties that are made by closing many thousands of plasmonic atoms and also photonic crystals with useful optical properties are alternative structures of photonic atoms [6].

As some properties of photonic molecules we can note to their frequency tune-ability and very small modal volume. We can engineer resonant frequencies of a photonic molecule by changing in atomicity and chromaticity and also the method of arranging them. For these molecules, significant application in various range of science have been prospected. Frequency tune-ability property of them can be used in controlled reaction of light-matter which has many uses in atomic physics and quantum optics ranges. Small modal volume of a photonic molecule smoothes the pathfor making micro lasers with ultra-small threshold [7], creating condensed optical states, increasing nonlinear property of nonlinear optical materials, and performing novel experiments in quantum physics range specially cavity quantum electrodynamics. One of the other effective applications of photonic molecules is related to cavity opto-mechanics [8]. Coupling of optical properties of photonic molecule with their mechanical properties provides a unique way for controlling and measurement of mechanical motion in micro and nano structures that can have great applications in lasers and novel filters and also processing of opto-mechanical signal. Also the proposal of making phonon lasers (PhASER) is considered as one of the other very modern topics of cavity opto-mechanics with photonic molecules [9,10].

In this paper resonant frequencies and optical modes of a linear three-atom photonic molecule and also photonic crystal that is placed in a cavity with conducting walls is computed in TE mode numerically. In the first part of the paper theory and algorithm used in paper are introduced. In the second part frequencies and resonant modes of three-atom photonic molecule inside the cavity are obtained. In the third part, frequencies and resonant modes of a photonic crystal that is placed in the cavity are computed. In the last part conclusion is drown.

2. Theoretical formulation and algorithm of numerical solution

Here a dielectric photonic molecule is considered and the governing formulation for resonant frequencies and related modes is presented.

2-1- Theoretical formulation

The photonic molecule is composed of cylindrical dielectric atoms with square cross-section with ε_a and μ_a in a medium with ε and μ, Fig. 1-a.

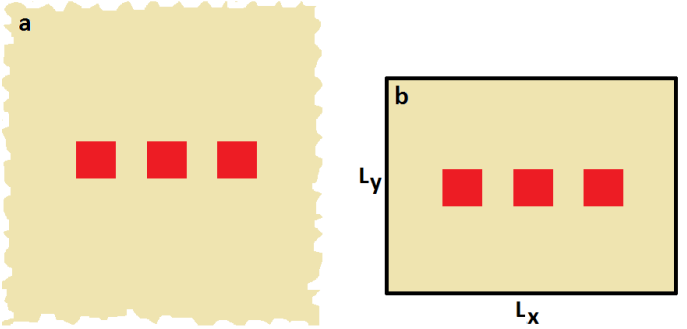

Fig. 1.(a) two-dimensional three-atom linear photonic molecule with square cross-section with ε_a and μ_a in a medium with ε and μ, (b) The same molecule in a square cavity.

Such a molecule can be considered in two different situations: 1) in a free space with no boundaries Fig. 1-a. 2) Placed in a bounded space or a cavity, Fig. 1-b. The first one is a scattering problem with no limit on the frequencies and the second one is a resonant problem with only a discrete number of frequencies. Here the second situation is considered and for simplicity a rectangular cavity with L_x and L_y is selected. Using Maxwell equations, one can find the resonant frequencies and related modes. The curl equations of Maxwell are:

$$\vec{\nabla}\times\vec{E}(\vec{r},t)=-\frac{\partial\vec{B}(\vec{r},t)}{\partial t},\ \vec{\nabla}\times\vec{B}(\vec{r},t)=\varepsilon\mu\frac{\partial\vec{E}(\vec{r},t)}{\partial t} \tag{1}$$

Mixing them yields:

$$\begin{aligned}\nabla^2\vec{E}(\vec{r},t)-\varepsilon\mu\frac{\partial^2\vec{E}(\vec{r},t)}{\partial t^2}=0\\ \nabla^2\vec{B}(\vec{r},t)-\varepsilon\mu\frac{\partial^2\vec{B}(\vec{r},t)}{\partial t^2}=0\end{aligned} \tag{2}$$

To solve Eq. 2, first of all, the polarization of the incident light should be selected. For simplicity, the TE polarization (i.e. electric field normal to page and magnetic field parallel with the page) is interested. The TM case is similar to TE one and is dropped here. For TE mode Eq. 2 converts to:

$$\begin{aligned}
\nabla^2 E_z(\vec{r},t) - \varepsilon\mu \frac{\partial^2 E_z(\vec{r},t)}{\partial t^2} = 0 \\
\nabla^2 B_x(\vec{r},t) - \varepsilon\mu \frac{\partial^2 B_x(\vec{r},t)}{\partial t^2} = 0 \\
\nabla^2 B_y(\vec{r},t) - \varepsilon\mu \frac{\partial^2 B_y(\vec{r},t)}{\partial t^2} = 0
\end{aligned} \tag{3}$$

With harmonic behavior of frequency ωand remembering that the problem is independent of z Eq. 3 yields:

$$\begin{aligned}
\nabla^2 E_z(x,y) + \omega^2 \varepsilon\mu E_z(x,y) = 0 \\
\nabla^2 B_x(x,y) + \omega^2 \varepsilon\mu B_x(x,y) = 0 \\
\nabla^2 B_y(x,y) + \omega^2 \varepsilon\mu B_y(x,y) = 0
\end{aligned} \tag{4}$$

To solve these eigenvalue equations the following boundary conditions should apply:

$$\begin{aligned}
E_{1t} = E_{2t},\ \varepsilon_1 E_{1n} = \varepsilon_2 E_{2n} \\
B_{1n} = B_{2n},\ \mu_2 B_{1t} = \mu_2 B_{2t}
\end{aligned} \tag{5}$$

Unfortunately, only for a few simple cases with analytical solutions, the Eqs. 4 and 5 must be solved numerically.

2-2- Algorithm of numerical solution

A simple finite difference scheme is used to solve Eq. 4 and 5.First, the molecule and computation space is divided to N differential squares with Δx and Δy, Fig. 2.

By a three-point algorithm of second order derivative in (i,j) square, Eq. 4 gets the discrete form of:

$$\begin{aligned}
&\frac{E_z(i+1,j) + E_z(i-1,j) - 2E_z(i,j)}{\Delta x^2} \\
&+ \frac{E_z(i,j+1) + E_z(i,j-1) - 2E_z(i,j)}{\Delta y^2} + \omega^2 \varepsilon\mu E_z(i,j) = 0 \\
&\frac{B_x(i+1,j) + B_x(i-1,j) - 2B_x(i,j)}{\Delta x^2} \\
&+ \frac{B_x(i,j+1) + B_x(i,j-1) - 2B_x(i,j)}{\Delta y^2} + \omega^2 \varepsilon\mu B_x(i,j) = 0 \\
&\frac{B_y(i+1,j) + B_y(i-1,j) - 2B_y(i,j)}{\Delta x^2} \\
&+ \frac{B_y(i,j+1) + B_y(i,j-1) - 2B_y(i,j)}{\Delta y^2} + \omega^2 \varepsilon\mu B_y(i,j) = 0
\end{aligned} \tag{6}$$

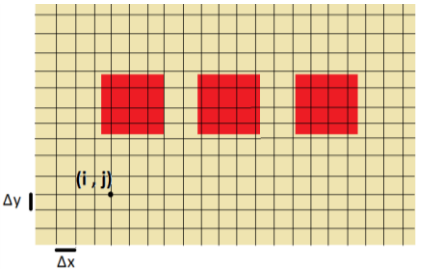

Fig. 2. Discretizingthemolecule and computation space toN differential squares of Δx and Δy.

Eq. 6 yields a set of three equations and three unknowns for each element (i,j), thus, for N elements, N equations and N unknowns for each field is finally obtained. Of course, ω is also unknown. As, all the equations are homogeneous, equating the coefficients matrix with zero yields the unknown ω. A massive Mathematica code is developed by the authorsthat solves numerically the problem and gives the resonant frequencies and fields. For typical N=10000, the run time is a fraction of hour by a home laptop of two CPUs with few GB of memory.

A linear three-atom molecule in the cavity

A photonic molecule with three square atoms of a=10 μm and $\varepsilon_a=10\varepsilon_0$ and $\mu_a=10\mu_0$ placed within a square cavity of $L_x=L_y=100\mu m$ with conducting walls is considered. Inside the cavity is vacuum with ε_0 and μ_0. For the configuration, the distribution of B_y field for three different equilateral, folded and linear configurations is shown in Fig. 3.

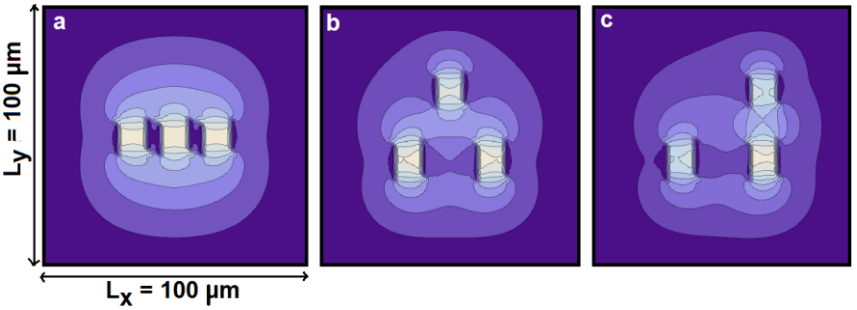

Fig. 3. Contour plots of distribution of B_y field within the cavityfor linear, a, equilateral, b, and folded, c, three-atom molecule. In bright regions field is stronger.

Here the linear case is interested and is studied with more details. In Fig. 4 the distribution of B_y field for a linear molecule from the most condensed case to the most expanded case is shown.

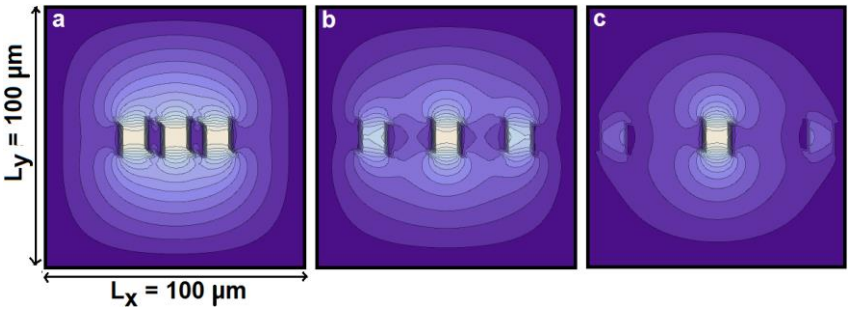

Fig. 4. The contour plot of B_y for a condensed molecule, a, for an intermediate molecule, (b), and for (a) expanded one, (c).

Fig. 4 clearly shows that, in the condensed case, the brightness of all atoms is equal. As long as the molecule is expanded, the lateral atoms become darker. This can be related to the effect of cavity walls. The resonant frequencies of the ground and the first excited states were calculated by the code as functions of the molecule length. In Fig. 5-b, the frequenciesare plotted. Figs. 5-a and 5-c are for $\varepsilon_a=5\varepsilon_0$ and $\mu_a=5\mu_0$ and also $\varepsilon_a=15\varepsilon_0$ and $\mu_a=15\mu_0$ cases, respectively.

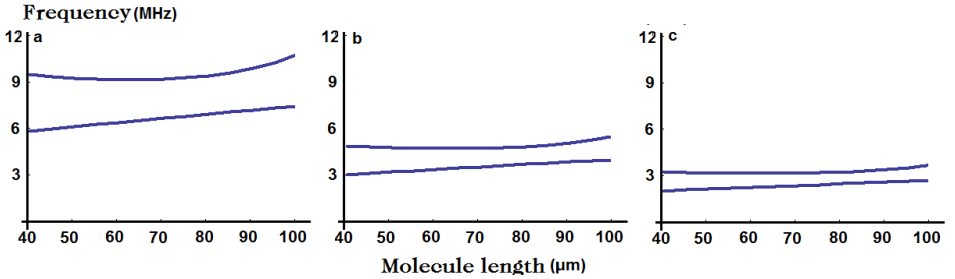

Fig. 5. The change of frequencies of ground and first excited states of a linear three-atom molecule with $\varepsilon_a=5\varepsilon_0$ and $\mu_a=5\mu_0$, (a), with$\varepsilon_a=10\varepsilon_0$ and $\mu_a=10\mu_0$, (b), and also with $\varepsilon_a=15\varepsilon_0$ and $\mu_a=15\mu_0$, (c), respectively.

The plots show that, with expansion of the molecule to a special length (here nearly 75 μm), independent of the optical constants, the ground state frequency is increased and the excited state frequency is decreased. After this special length, the ground frequency remains fixed and the excited one's starts increasing. Such a behavior can be related to the cavity walls. As long as the cavity walls are far and have no effect, the frequency difference of ground and excited states is decreased by expanding. This is a known effect and is reasonable because expanding the molecule in a free space leads to developing the degeneracy and hence decreasing of frequency differences [1]. On the other hand, the calculations show that, interaction with cavity walls removes the degeneracy and leads to increasing frequency differences.

Photonic crystal within the cavity

In continuation, we investigate theresonantfrequencyandfield distributionofa pieceofphotoniccrystallocated within anexternalcavity.Fig.6showsan overviewof the situation.Thecode was conductedforthe case ofaphotoniccrystalwith asquarebaseof side length a= 10 µm and with lattice constant of L= 20 µm that completelyfills internal space of a rectangularcavity with sides L_y= L_x= 100µm.

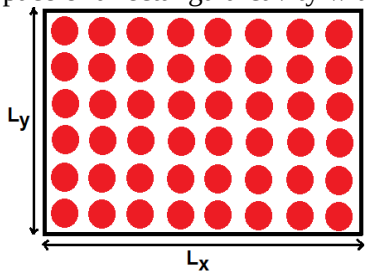

Fig. 6. Schemas of a photonic crystal that is located inside a rectangular cavity.

InFig.7 the ground state field distribution and the firstexcited statefield distribution were drawn.This plot indicates that the densitydistribution ofthe ground statein thecentral region ofthe cavity is high.Forthe firstexcited state, thefield distributionin bothleft and right sections issymmetric.Thesedistributionsarevery similar to thedistributionwhenall the inner space of cavityisuniformly filled.However, in higherresonantfrequencies this similaritydisappears.Thisshows thata photoniccrystal in the ground stateand the firstexcited statewith low frequencies(the higherwavelengths) behavelike a cavitywhich is completely filled with a homogeneous material with effective indices.

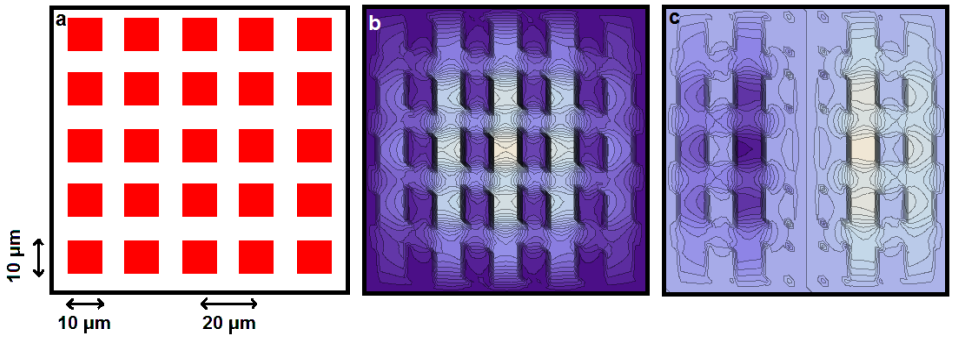

Fig. 7.Photoniccrystalwitha squarelattice with lattice constant L= 20 µm and squarebasewith side a= 10 µm that fillscompletely (a) rectangularcavity with sides L_y= L_x= 100µm, a. In figure (b), the ground state field distribution, and in figure (c), the firstexcited statefield distribution were drawn.

At the end,the trend of the frequency changing oftheground state and the firstexcited state ofthe photoniccrystal as functions of permittivityandpermeabilitycoefficientsisobtained and plottedin Fig. 8.

Calculations show that independent ofthephotoniccrystalopticalconstantsand thesurrounding space theresonantfrequenciesand the differencebetween themis reduced.This phenomenonusing the relation νλ=c/nwherec is the speedof light in vacuum, n the refractive indexofthecavity, λwavelength, and ν isthe frequency is justifiable. Accordingto itfor twoequal wavelengths, thefrequencyin the cavitywith higher n is smaller.

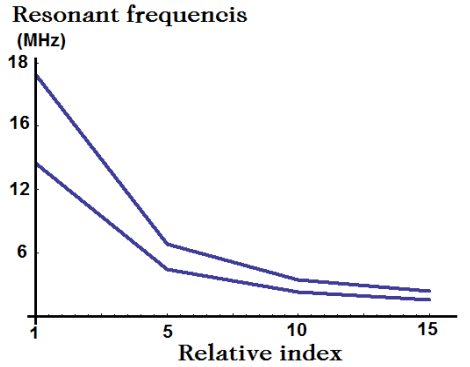

Fig. 8. The trend of frequency changing of the ground state and the first excited state of the photonic crystal in the cavity as functions if permittivity and permeability coefficients.

3. Conclusion

In the paper, the problem of calculation of resonant frequencies and related modes of a linear three-atomic photonic molecule placed within a cavity was considered for the first time. Using a massive computer code developed by the authors, problem was numerically solved. Calculations show that increasing the molecule length to a special one, the frequencies come closer to each other. Beyond that length, a reverse event is occurred. It can be related to the cavity walls. For small length, the walls have no effect and the molecule behavior is like a free molecule and increasing the length leads to developing degeneracy and decreased difference of frequencies. But, beyond the special length, the walls perturb the problem and remove the degeneracy. Generalizing the simulation to the case of a larger cavity for considering the interaction of two or more molecules is remained as a future work.

For the case where the cavity is filled with a photonic molecule, calculations show that field distributions (e.g. for ground and first excited states) are similar to the case where the cavity is filled with a homogeneous medium. It reveals that, for longer wavelengths photonic crystal behaves like a homogeneous medium with effective indices. On the other hand, by increasing the indices, the

space between frequencies is decreased. This phenomenon is justifiable by $c/n = \nu\lambda$ which says that cavities with higher values of indices have lower frequencies in equal wavelengths. Calculation of wall effects on optical band gap and its change in terms of crystal parameters is another future work of the authors.

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