Polariton Modes in Two-Dimensional Dispersive and Absorptive Photonic Crystals

N.Chandrasekar

*Abstract***: *Two-dimensional photonic crystals play important role in practical photonic devices. In this study, Hamiltonian method is used to determine the evolution equations for the fields. This method allows us to determine the polariton modes inside a periodically structured medium. For a two-dimensional photonic crystal, the Hamiltonian for electromagnetic field interaction with structured medium is constructed and the evolution equations for fields are determined from Hamilton's equations of motion. The polariton modes are found from the canonical form of the Hamiltonian.*

*Keywords***: *Hamiltonian, Photonic Crystals, Polariton, Structured Medium*

I. INTRODUCTION

Periodically structured dielectric media are artificially created materials through which the electromagnetic wave propagation shows properties that are generally not found in the natural materials. They are known as photonic crystals and consist of periodically repeated unit cell structure in one, two, or three dimensions [1-6]. The properties of the photonic crystals are determined by the nature and the distribution of the constituent materials in the unit cell structure. In photonic crystals the linear dimension of the unit cell is comparable to the operating wavelength and the periodic structure act as periodic potential for the wave giving rise to unusual properties [7-10]. These strange properties have many potential applications like perfect lens [11], cloaking [12], and other novel electromagnetic devices. The important property of the photonic crystals is the Photonic Band Gap (PBG) because of which the electromagnetic waves of certain frequency ranges cannot exist inside the photonic crystals. This gives rise to the property of localization of the radiation in a point defect in the photonic crystal and the property of bandgap guidance of the radiation inside a line defect in the two-dimensional photonic crystal. This improved control over the radiation in the photonic crystals promises novel photonic devices. Most of the studies of the structured media are done with the modal values of the dielectric function without considering the dispersive and absorptive characteristics.

In any realistic study of the structured media the dispersion and the absorption must be included to get the full picture of the phenomenon [13-15]. In some applications the absorption and the dispersion are used for the effective device performance and in other cases, they become undesirable [11,12,14,16]. So, the inclusion of the dispersion and the absorption of the structured media becomes very important in any realistic study of these materials for applications [17].

In this study, we apply the Hamiltonian approach to find the polariton mode field in a two-dimensional photonic crystal. These structures are of practical importance because of their potential applications in all-optical passive and active devices in the field of optical communication and signal processing. Light propagation through a defect line in the two-dimensional photonic crystal which occurs due to Band-Gap Guidance allows us to control the light more efficiently than the conventional index guidance of the light. We consider a photonic crystal with a two-dimensional array of cylindrical rods in air and also with a two-dimensional array of cylindrical holes filled with air in a dielectric medium. The wave propagation consists of both the Transverse Magnetic (TM) and the Transverse Electric (TE) modes. The total Hamiltonian consists of three parts, namely, the Hamiltonian of electromagnetic field in free space, the Hamiltonian of the medium and the interaction Hamiltonian which describes the interaction between the electromagnetic waves and the medium. For the two-dimensional structured medium, the dielectric function in the medium Hamiltonian is expanded as two-dimensional Fourier series and a solution is sought for the medium oscillator operators through Hamilton's equations for the medium oscillators. The total Hamiltonian is expressed in terms of the Fourier series of the dielectric function, the electric and the magnetic fields. The final solution for the fields is determined from the Hamilton's equations of motion using the electric displacement field, $\mathbf{D}$ and magnetic flux density, $\mathbf{B}$ as the dynamical variables in the total Hamiltonian.

II. HAMILTONIAN FOR ELECTROMAGNETIC FIELD IN TWO DIMENSIONAL DISPERSIVE AND ABSORPTIVE STRUCTURED DIELECTRIC MEDIUM

The Hamiltonian for electromagnetic field interacting with medium consists of three parts. The first part gives the Hamiltonian of the field in free space, the second part gives the Hamiltonian of the medium considering the medium as continuum of harmonic oscillators and the third part gives interaction

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648

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Hamiltonian which accounts for the interaction between the field and the medium. The general form of the Hamiltonian for the electromagnetic interaction with the structured medium is given as [18]

$$H = \frac{1}{2\mu_0}\int dV \mathbf{B}(\mathbf{r})\cdot\mathbf{B}(\mathbf{r}) + \frac{1}{2\varepsilon_0}\int dV \mathbf{D}(\mathbf{r})\cdot\mathbf{D}(\mathbf{r}) +$$

$$\int dV \int d\Omega \hbar\Omega b^\dagger(\mathbf{r},t)b(\mathbf{r},t)$$

$$-\int dV \int d\Omega \sqrt{\frac{\hbar}{2\varepsilon_0\Omega}}\mathbf{D}(\mathbf{r},t)\cdot\Lambda(\mathbf{r},\Omega)\cdot\big(b(\mathbf{r},t)+b^\dagger(\mathbf{r},t)\big)$$

$$(1)$$

with the equal-time commutator relations for the fields

$$\left[D^i(\mathbf{r}),\quad D^j(\mathbf{r}')\right]=\left[B^i(\mathbf{r}),\quad B^j(\mathbf{r}')\right]=0$$

$$\left[D^i(\mathbf{r}),\quad B^j(\mathbf{r}')\right]=i\hbar\varepsilon^{ilj}\frac{\partial}{\partial r}\left[\delta(\mathbf{r}-\mathbf{r}')\right]$$

$$(2)$$

and for the medium oscillator operators

$$\left[b_\Omega(\mathbf{r})\quad b_{\Omega'}^\dagger(\mathbf{r}')\right]=\delta(\mathbf{r}-\mathbf{r}')\delta(\Omega-\Omega')$$

$$(3)$$

The dynamical equations for the fields are

$$i\hbar\frac{\partial \mathbf{D}}{\partial t}=\left[\mathbf{D},\quad H\right]$$

$$i\hbar\frac{\partial \mathbf{B}}{\partial t}=\left[\mathbf{B},\quad H\right]$$

$$(4)$$

and for the medium field operators are

$$i\hbar\frac{\partial b}{\partial t}=\left[b,\quad H\right]$$

$$i\hbar\frac{\partial b^\dagger}{\partial t}=\left[b^\dagger,\quad H\right]$$

$$(5)$$

We consider a photonic crystal with dielectric value of the medium varying along x- and y-directions and variation along z-direction. If the electric field is along the z-direction with magnetic field in x-y plane then it is known as Transverse Magnetic Mode or TM mode, and if the electric field in x-y plane then it is known as Transverse Electric Mode or TE mode.

III. TE MODE

For the two-dimensional photonic crystal, the dielectric function is expanded in Fourier series. The Fourier expansion can be determined from the wave equation for magnetic field through the photonic crystal [19]. The magnetic field and the dielectric function are expanded by double Fourier series and substituted in the wave equation. Integrating over one period and comparing terms on both sides we arrive at the double Fourier series expansion for the two-dimensional photonic crystal. For TE mode the wave equation for magnetic field is

$$\nabla\times\left[\frac{1}{\varepsilon_r(x,y)}\nabla\times\hat{\mathbf{z}}H_z(x,y)\right]+k_0^2\hat{\mathbf{z}}H_z(x,y)=0 \qquad (6)$$

where $\varepsilon_r(x,y)$ is relative permittivity which varies along both x- and y- directions. Expanding the wave equation operator in Eq. (4.6) we get

$$\frac{1}{\varepsilon_r(x,y)}\hat{\mathbf{z}}\cdot\nabla\times\nabla\times\mathbf{H}(x,y) +$$

$$\hat{\mathbf{z}}\cdot\nabla\left[\frac{1}{\varepsilon_r(x,y)}\right]\times\nabla\times\mathbf{H}(x,y)=-k_0^2 H_z(x,y)$$

$$(7)$$

In x-y plane the shape of unit cell is a square side a and the cross section of the dielectric rod in x-y plane has the diameter b.
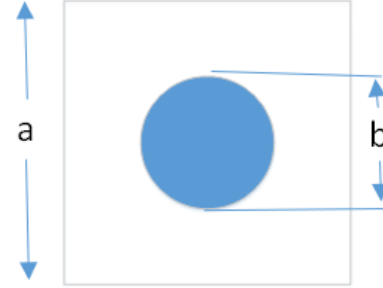

Fig. 1 Unit Cell Consisting of Square Cell with Cylindrical Dielectric at Center

Expanding the magnetic field and the dielectric function in periodic functions [20]

$$H(x,y)=\sum_n\sum_q a_{nq}e^{-j\frac{2\pi n}{a}x}e^{-j\frac{2\pi q}{c}y} \qquad (8)$$

$$\frac{1}{\varepsilon_r(x,y)}=\sum_m\sum_p b_{mp}e^{-j\frac{2\pi m}{a}x}e^{-j\frac{2\pi p}{a}y} \qquad (9)$$

and substituting in Eq. (4.7) and evaluating the vector operators

$$\sum_m\sum_p b_{mp}e^{-j\frac{2\pi m}{a}x}e^{-j\frac{2\pi p}{a}y}\left[-\frac{\partial^2}{\partial x^2}\sum_n\sum_q a_{nq}e^{-j\frac{2\pi m}{a}x}e^{-j\frac{2\pi q}{c}y}e^{-jk_{x0}x}e^{-jk_{y0}y}\right.$$

$$-\frac{\partial^2}{\partial y^2}\sum_n\sum_q a_{nq}e^{-j\frac{2\pi m}{a}x}e^{-j\frac{2\pi q}{c}y}e^{-jk_{x0}x}e^{-jk_{y0}y}\Bigg]$$

$$-\frac{\partial}{\partial x}\sum_m\sum_p b_{mp}e^{-j\frac{2\pi m}{a}x}e^{-j\frac{2\pi p}{a}y}\frac{\partial}{\partial x}\sum_n\sum_q a_{nq}e^{-j\frac{2\pi n}{a}x}e^{-j\frac{2\pi q}{c}y}e^{-jk_{x0}x}e^{-jk_{y0}y}$$

$$-\frac{\partial}{\partial y}\sum_m\sum_p b_{mp}e^{-j\frac{2\pi m}{a}x}e^{-j\frac{2\pi p}{a}y}\frac{\partial}{\partial y}\sum_n\sum_q a_{nq}e^{-j\frac{2\pi n}{a}x}e^{-j\frac{2\pi q}{c}y}e^{-jk_{x0}x}e^{-jk_{y0}y}$$

$$=-k_0^2\sum_n\sum_q a_{nq}e^{-j\frac{2\pi n}{a}x}e^{-j\frac{2\pi q}{c}y}e^{-jk_{x0}x}e^{-jk_{y0}y}$$

$$(10)$$

Simplifying the above expression and integrating over a unit cell yield an equation

$$\sum_m\sum_p a_{nq}b_{n-m,q-p}\left[\begin{array}{c}\left(\frac{2\pi n}{a}+k_{x0}\right)^2+\left(\frac{2\pi q}{a}+k_{y0}\right)^2 \\ -\frac{2\pi(n-m)}{a}\left(\frac{2\pi n}{a}+k_{x0}\right)-\frac{2\pi(q-p)}{c}\left(\frac{2\pi q}{a}+k_{y0}\right)\end{array}\right]=-k_0^2 a_{nq}$$

$$(11)$$

The Fourier coefficient for the cylindrical rods is

$$b_{n-m,q-p} = \frac{\pi b^2}{a^2}\left(\frac{1}{\varepsilon_r}-1\right)$$

$$\frac{2J_1\left(\sqrt{\left(\frac{2\pi(n-m)b}{a}\right)^2+\left(\frac{2\pi(q-p)b}{a}\right)^2}\right)}{\sqrt{\left(\frac{2\pi(n-m)b}{a}\right)^2+\left(\frac{2\pi(q-p)b}{a}\right)^2}}+\delta_{n-m,q-p}$$

$$(12)$$

To get compact notation the indices can be renamed as $n-m\to m$ and $q-p\to p$ to get

$$b_{m,p} = \frac{\pi b^2}{a^2}\left(\frac{1}{\varepsilon_r}-1\right)\frac{2J_1\left(\sqrt{\left(\frac{2\pi mb}{a}\right)^2+\left(\frac{2\pi pb}{a}\right)^2}\right)}{\sqrt{\left(\frac{2\pi mb}{a}\right)^2+\left(\frac{2\pi pb}{a}\right)^2}}+\delta_{m,p}$$

$$(13)$$

which can be substituted in the Eq. (9). The coupling factor of the interaction Hamiltonian in Eq. (1) can be given as

$$\Lambda(\mathbf{r},\Omega) = \sqrt{\frac{2\Omega}{\pi}\text{Im}\left(1-\frac{\varepsilon_0}{\varepsilon(\mathbf{r},\Omega)}\right)} \qquad (14)$$

for isotropic dielectric medium. Here Im(...) means that imaginary part of (...) is taken. For photonic crystal with array of cylindrical dielectric rods in air medium can be given as

$$\Lambda(\mathbf{r},\Omega) = \sqrt{\frac{2\pi}{\Omega}\text{Im}\left(1-\sum_m\sum_p b_{mp}e^{-j\frac{2\pi m}{a}x}e^{-j\frac{2\pi p}{a}y}\right)}$$

$$(15)$$

Once the coupling factor is determined, the equations of motion for the field operators b_Ω and $b_\Omega^\dagger$. This can be achieved by constructing the total Hamiltonian and solving the Hamilton's equations for the field operators. The total Hamiltonian is

$$H = H_{em} + H_{med} + H_{int} \qquad (16)$$

$$H = \frac{1}{2\mu_0}\int dVB^2(x,y,t) + \frac{1}{2\varepsilon_0}\int dVD^2(x,y,t)$$

$$+ \int d\Omega\int dV \hbar\Omega b^\dagger(x,y,t)b(x,y,t)$$

$$- \int d\Omega\int dV \sqrt{\frac{\hbar}{2\varepsilon_0\Omega}}D(x,y,t)$$

$$\Lambda(x,y,t)\left(b^\dagger(x,y,t)+b(x,y,t)\right)$$

$$(17)$$

with the equal-time commutator relation

$$\left[b_\Omega(x,y),\ b_{\Omega'}^\dagger(x,y)\right] =$$
$$\delta(x-x')\delta(y-y')\delta(\Omega-\Omega') \qquad (18)$$

The Hamilton's equations of motion for the field operators are

$$i\hbar\frac{db}{dt} = [b,\ H]$$
$$i\hbar\frac{db^\dagger}{dt} = [b^\dagger,\ H] \qquad (19)$$

In explicit form

$$\frac{db}{dt} = -i\Omega b + i\sqrt{\frac{1}{2\varepsilon_0\hbar\Omega}}D(x,y,t)\Lambda(x,y,\Omega)$$

$$\frac{db^\dagger}{dt} = i\Omega b^\dagger + i\sqrt{\frac{1}{2\varepsilon_0\hbar\Omega}}D(x,y,t)\Lambda(x,y,\Omega)$$

$$(20)$$

Integration of the Eqs. (20) consists of the term with integration constant which corresponds to the motion of the medium oscillators without the external electromagnetic fields. As it corresponds to the thermal motion of the oscillators at a given temperature, the average value of it becomes zero over a period of time, long enough for many periods of oscillations and at the same time, short enough in macroscopic scale. Neglecting the term with integration constant, the solution for the field operators can be given as

$$b(x,y,t) = \sqrt{\frac{1}{2\varepsilon_0\hbar\Omega}}\frac{D(x,y)\Lambda(x,y,\Omega)}{(\Omega+\omega)}e^{i\omega t} \qquad (21)$$

$$b^\dagger(x,y,t) = \sqrt{\frac{1}{2\varepsilon_0\hbar\Omega}}\frac{D(x,y)\Lambda(x,y,\Omega)}{(\Omega-\omega)}e^{i\omega t} \qquad (22)$$

In the above solution, Eqs. (21), and (22), we assumed harmonic variation of electric displace vector

$$D(x,y,t) = D(x,y)e^{i\omega t} \qquad (23)$$

By substituting Eqs. (21) and (22) in the expression for the Hamiltonian, Eq. (17) we get a function which depends only on $D(x,y,t)$, $B(x,y,t)$ and $\Lambda(x,y,\Omega)$. The total Hamiltonian is

$$H = \frac{1}{2\mu_0}\int dxdyB^2(x,y) + \frac{1}{2\varepsilon_0}\int dxdyD^2(x,y)$$

$$- \int dxdy\int d\Omega\left(\frac{1}{2\varepsilon_0}\right)\frac{D^2(x,y)\Lambda^2(x,y)}{(\Omega^2-\omega^2)}$$

$$(24)$$

The Hamiltonian can be rewritten as

$$H = \frac{1}{2\mu_0}\int dxdyB^2(x,y) +$$

$$\frac{1}{2\varepsilon_0}\int dxdyD^2(x,y)\left\{1+\int d\Omega\frac{\Lambda^2(x,y)}{(\omega^2-\Omega^2)}\right\}$$

$$(25)$$

$$H = \frac{1}{2\mu_0}\int dVB^2 + \frac{1}{2\varepsilon_0}\int dVD_p^2$$

$$(26)$$

where the electric displacement vector for the polariton mode, $D_p(x,y,t)$, can be given as

$$D_p^2 = D^2(x,y)$$

$$\left\{1+\int d\Omega\frac{\frac{2\Omega}{\pi}\text{Im}\left(1-\sum_{m,p}b_{mp}e^{-i\frac{2\pi m}{a}x}e^{-i\frac{2\pi p}{a}y}\right)}{(\omega^2-\Omega^2)}\right\}^{1/2} \qquad (27)$$

The equation Eq. (27) indicates the modification in the electric displacement vector in the medium due the presence of external electromagnetic fields.

The Eq. (26) can be considered as the Hamiltonian of the polariton mode in a two-dimensional structured medium where the structure information is included in the coupling term, $\Lambda(x,y,\Omega)$ as given the Eq. (15).

IV. EXAMPLE

As an example of determining the electric displacement vector in a two-dimensional photonic crystal, we consider a two-dimensional array of dielectric cylinders in a air medium. The unit cell of this photonic crystal is as shown in the Fig.1 and the lattice size taken as $2\mu m$. The dielectric is GaAs whose permittivity data is given Fig.2. The ratio of diameter of the cylinder to the side of the square lattice is taken as

$$\frac{b}{a} = 0.4$$

and the Fourier coefficients are taken up to second order as

$$b_{00} = 0$$
$$b_{-1-1} = b_{11} = b_{-11} = b_{1-1} = 0.884642$$
$$b_{-2-1} = b_{21} = b_{2-1} = b_{-21} = 0.049536$$
$$b_{-1-2} = b_{12} = b_{1-2} = b_{-12} = 0.049536$$

Polariton field distribution at frequency, $\omega = 5$ units is determined which is shown in Fig 2. Consider a dielectric medium that has the constant complex dielectric response over a frequency range 0 to Ω_0. The constant complex dielectric response is given by the coupling constant Λ_0. The electric displacement for the polariton mode can be given as

$$D_p =$$
$$D\left\{ 1 + \Lambda_0^2 \frac{(e^{i\omega t} - e^{-i\Omega_0 t})(e^{i\Omega_0 t} - e^{i\omega t})}{\omega} \tanh^{-1}\left(\frac{\Omega_0}{\omega}\right) \right.$$
$$\left. + \frac{\Omega_0 \Lambda_0^2}{\omega}\left(\frac{(e^{i\omega t} - e^{-i\Omega_0 t})}{(\omega + \Omega_0)} + \frac{(e^{i\Omega_0 t} - e^{i\omega t})}{(\omega - \Omega_0)} \right) \right\}$$

(28)

For two-dimensional structured medium the coupling term can be function of two coordinates, x, and y. Thus

$$D_p =$$
$$D\left\{ 1 + \Lambda_0^2(x,y) \frac{(e^{i\omega t} - e^{-i\Omega_0 t})(e^{i\Omega_0 t} - e^{i\omega t})}{\omega} \tanh^{-1}\left(\frac{\Omega_0}{\omega}\right) \right.$$
$$\left. + \frac{\Omega_0 \Lambda_0^2(x,y)}{\omega}\left(\frac{(e^{i\omega t} - e^{-i\Omega_0 t})}{(\omega + \Omega_0)} + \frac{(e^{i\Omega_0 t} - e^{i\omega t})}{(\omega - \Omega_0)} \right) \right\}$$

(29)

Eq. (29) represents the magnitude of electric displacement vector of a polariton mode in a two dimensional periodically structured medium. The structure is analytically represented in the two-dimensional coupling factor $\Lambda(x,y)$. The first term in curly bracket in Eq. (29) with $D(x,y)$ multiplied from outside the bracket represents the field in the medium without dispersion and absorption. The value of $D(x,y)$ can be directly determined from Maxwell's equations in homogenous medium without dispersion and absorption. The polariton field can be determined from Eq. (29). It can be clearly seen that the field distribution is modified in presence of dispersion and absorption.

When the photon enters the medium, the electric field polarizes the atoms in the medium and a combined state of electromagnetic field of the photon and the medium polarization exists inside the medium. This is similar to the coupled oscillations of two pendulums with different frequencies. When coupled, it will oscillate with new eigenfrequencies.

The polarization oscillations can propagate as both longitudinal and transverse waves through the medium. This forms the polariton modes in the medium. In quantum mechanical case, interaction between light and Frenkel-excitons produces bound states. This new stationary state has new energies and a new law of dispersion which corresponds to the polariton mode.
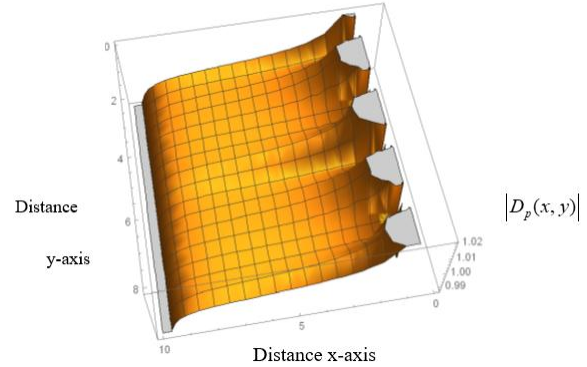

Fig.2. Magnitude of Electric Displacement Vector in Two-Dimensional Structured Medium consisting of cylindrical rods periodically arranged to form Two-Dimensional Crystal.

The z-axis in Fig.2, shows the magnitude of the electric displacement field of the polariton mode $|D_p(x,y)|$ which in general is different when usual Maxwell's equations are considered. It is the polariton modes which actually exists inside the medium when a photon enters the medium.

V. CONCLUSION

Hamiltonian for electromagnetic interaction with a two-dimensional photonic crystal containing periodic array of cylindrical dielectric rods is constructed. The evolution equations for the electric and magnetic fields are determined from the Hamilton's equations of motion. The polariton modes obtained from the canonical form of Hamilton's equations of motion. The electric field inside the structured medium for a polariton mode is determined.

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651

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