行政院國家科學委員會專題研究計畫

RRPA89020070 (5.P)

計畫編號：NSC 89-2112-M-034-001

執行期限：88 年 8 月 1 日至 89 年 7 月 31 日

主持人：程思誠 (Email:sccheng@faculty.pccu.edu.tw) 中國文化大學物理系

一、中文摘要

利用有效質量法吾人可以了解電磁波在光晶體內傳遞的特性，經由研究電磁波在光能隙附近的傳遞，吾人發現電磁波的傳遞可以由具質量且帶電的質點運動來描述，此質點的自旋為 0，而此質點的運動具有相對論效應，這相對論效應與電磁波的傳遞本身既具有相對論效應彼此吻合，電磁波在光能隙附近的傳遞與在均勻介質內傳遞的特性完全不同，電磁波既帶電又具質量，使得吾人相信電磁波在光晶體內轉變為一新的基本粒子，此粒子為帶電且自旋為 0 的質點。

關鍵詞：電磁波、光能隙、相對論效應

Abstract

Using the **k • p** theory, we have derived the Klein-Gordon equation to describe the EM wave propagating in photonic crystals. We find that the EM field posses an effective mass, which is the photon energy, divided by square of the effective speed of light. The EM field is a massive vector field in photonic crystals. The transverse and longitudinal modes of a massive vector field are coupled. The EM wave propagating in the photonic crystal possesses a relativistic effect.

Keywords: EM wave, Photonic crystal, Relativistic effect.

二、緣由與目的

The problem of propagation of waves in multicomponent composites has attracted much attention in the past years. The periodic dielectric structures of three dimensions were proposed as means of providing greater control over the dispersion of the electromagnetic (EM) field [1]. The material structure, that posses the periodic dielectric structure is called the photonic crystals. When the dielectric contrast, i.e., the ratio of the dielectric constants of the different materials in the crystal, becomes large enough, then the dispersion of the EM waves can have novel and interesting features due to strong interference and diffraction. It has been observed experimentally that there exist ranges of frequencies in which propagation of EM waves is not allowed [2]. These frequency ranges are termed "photonic band gaps" in analogy with the electronic band gaps in solids. Many optical and microwave devices are now being designed based on the existence of such photonic band gaps.

Photonic band structures have been calculated for different systems in 1-3 dimensions using various traditional electronic band structure techniques including plane wave expansion [2] and Green's function method [3]. However, these techniques are highly computationally intensive. The **k • p** theory [4] has been proved to be a simple and successful method for describing various electronic properties in ordered and disordered semiconductors, without the need for full-scale numerical calculations. The technique leads to the f-sum rule relating the effective mass of a band to the coupling between energy bands and the energy separation between bands. This method has been extended to study semiconductor superlattices with great success. Johnson and Hui [5] have proposed using **k • p** extension to the scalar EM problem. An effective dielectric tensor is defined. The scalar wave function is appropriate for certain structures, which preserve a definite polarization, and to other physical problems in acoustics [6]. It is entirely inadequate in predicting even qualitatively correct results for dielectric materials with periodicity in all three dimensions. The appropriate EM equation for studying the photonic crystal should be a hermitian vector equation proposed by Ho *et al* [2].

Starting from Maxwell's equations, by eliminating the electric field, Ho *et al* obtain, for a monochromatic wave of frequency ω, the following hermitian equation for the magnetic field:

$$\nabla \times [\frac{1}{\varepsilon(r)} \nabla \times]\, \mathbf{H} = \frac{\omega^2}{c^2} \mathbf{H}, \qquad (1)$$

where $\varepsilon(\mathbf{r})$ is the dielectric constant and c is the vacuum speed of light. Applications of Eq. (1) are just like the applications of Schrödinger equation in semiconductor. We have derived an effective dielectric tensor equation that has a similar structure of the effective-mass equation in semiconductor and can be written as

$$\left(\frac{1}{\varepsilon^*}\right)_{\alpha\beta} = \lambda_{nn}(\mathbf{k}_0)\delta_{\alpha\beta} - \frac{1}{2} q_{nn}^{\alpha\beta}(\mathbf{k}_0) - \frac{1}{2} q_{nn}^{\beta\alpha}(\mathbf{k}_0) + \frac{1}{8}\sum_j \frac{\pi_{nj}^{\beta}(\mathbf{k}_0)\pi_{nj}^{\alpha}(\mathbf{k}_0) + \pi_{nj}^{\alpha}(\mathbf{k}_0)\pi_{nj}^{\beta}(\mathbf{k}_0)}{\Lambda_n(\mathbf{k}_0) - \Lambda_j(\mathbf{k}_0)} \qquad (2)$$

where $\Lambda=(\hbar\omega)^2/c^2$ and n, j are band indices. Define the volume of the first Brillouin zone as Ω and the Kohn-Luttinger function $\frac{1}{\sqrt{\Omega}}\mathbf{u}_j(\mathbf{k}_0,\mathbf{r})e^{i\mathbf{k}.\mathbf{r}}$, where $\mathbf{k}_0$ is some fixed **k** vector within the first Brillouin zone. The function $\mathbf{u}_j(\mathbf{k}_0,\mathbf{r})$ is periodic in **r** with the same periodicity as $\varepsilon(\mathbf{r})$. We have the matrices:

$$\lambda_{ij}(\mathbf{k}_0) = \frac{(2\pi)^3}{\Omega}\int_\Omega \frac{1}{\varepsilon(\mathbf{r})}\mathbf{u}_i^*(\mathbf{k}_0,\mathbf{r}) \bullet \mathbf{u}_j(\mathbf{k}_0,\mathbf{r})d\mathbf{r}$$

$$q_{ij}^{\alpha\beta}(\mathbf{k}_0) = \frac{(2\pi)^3}{\Omega}\int_\Omega \frac{1}{\bar{\varepsilon}(\mathbf{r})} u_i^{\alpha}(\mathbf{k}_0,\mathbf{r}) \bullet u_j^{\beta}(\mathbf{k}_0,\mathbf{r})d\mathbf{r},$$

$$P_{ij}^{\alpha}(\mathbf{k}_0) = \frac{(2\pi)^3}{\Omega}\int_\Omega \mathbf{u}_i^*(\mathbf{k}_0,\mathbf{r}) \bullet \left[\left(\frac{\hbar}{i}\nabla_\alpha\right)\left(\frac{1}{\varepsilon(\mathbf{r})}\mathbf{u}_j(\mathbf{k}_0,\mathbf{r})\right)\right]d\mathbf{r},$$

$$U_{ij}^{\alpha}(\mathbf{k}_0) = \frac{(2\pi)^3}{\Omega}\int_\Omega u_i^{\alpha *}(\mathbf{k}_0,\mathbf{r})\left[\left(\frac{\hbar}{i}\nabla\frac{1}{\varepsilon(\mathbf{r})}\right) \bullet \mathbf{u}_j(\mathbf{k}_0,\mathbf{r})\right]d\mathbf{r},$$

$$V_{ij}^{\alpha}(\mathbf{k}_0) = \frac{(2\pi)^3}{\Omega}\int_\Omega \frac{1}{\varepsilon(\mathbf{r})} u_i^{\alpha *}(\mathbf{k}_0,\mathbf{r})\left[\frac{\hbar}{i}\nabla \bullet \mathbf{u}_j(\mathbf{k}_0,\mathbf{r})\right]d\mathbf{r},$$

$$\pi_{ij}^{\alpha}(\mathbf{k}_0) = P_{ij}^{\alpha}(\mathbf{k}_0) + L_{ij}^{\alpha}(\mathbf{k}_0) - U_{ij}^{\alpha}(\mathbf{k}_0) - V_{ij}^{\alpha}(\mathbf{k}_0)$$

and

$$\mathbf{L}_{ij}^{\alpha}(\mathbf{k}_0)=\frac{(2\pi)^3}{\Omega}\int_{\Omega}\frac{1}{\varepsilon(\mathbf{r})}\mathbf{u}_i^*(\mathbf{k}_0,\mathbf{r})\times\frac{\hbar}{i}\nabla\times\mathbf{u}_j(\mathbf{k}_0,\mathbf{r})d\mathbf{r}$$

From the effective-dielectric equation, we can use the $\mathbf{k}\bullet\mathbf{p}$ theory to study the EM waves propagating near the photonic band gap without laborious calculations. The $\mathbf{k}\bullet\mathbf{p}$ theory can be applied to problems with disorder and nonlinear response to examine the wave propagation in a perturbed medium without the need for numerical calculations of the whole band structure.

Using the effective-dielectric tensor of Eq. (2), the hermitian Eq. (1) can be written as an eigenvlaue equation:

$$[(\frac{\hbar\omega_n(\mathrm{q})}{c})^2-(\frac{\hbar\omega}{c})^2]C_n(\mathrm{q})=0, \qquad (3)$$

where

$$(\frac{\hbar\omega_n(\mathrm{q})}{c})^2=(\frac{\hbar\omega_n(\mathrm{q}_0)}{c})^2+\hbar^2\sum(\frac{\varepsilon}{\varepsilon^*})_{ij}S_iS_j$$

and $\mathbf{S}=\mathbf{q}\text{-}\mathbf{q}_0$. Eq. (3) is the well-known effective-mass equation, written, however, in "momentum" space. To get more useful formulation, we introduce an envelope function

$$\mathrm{F}_n(r)=\int e^{iS\bullet r}C_n(q)d^3q,$$

the integration being over the first Brillouin zone. Thus, we have

$$[(\frac{\hbar\omega_n(q_0)}{c})^2+\hbar^2\sum(\frac{1}{\varepsilon^*})_{ij}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}]F_n(r)=(\frac{\hbar\omega}{c})^2F_n(r) \qquad (4)$$

where i and j are indices of three different directions of $\mathbf{r}$. We can also transform Eq. (4) back to the time space to study the temporal evolution of $F(\mathbf{r}, t)$. We have a tensor equation:

$$[\frac{\hbar^2\tilde{\varepsilon}^*}{c^2}\frac{\partial^2}{\partial t^2}-\hbar^2\nabla\bullet\tilde{I}\bullet\nabla+(\frac{\hbar\omega_n(q_0)}{c})^2\tilde{\varepsilon}^*]F_n(r,t)=0 \qquad (5)$$

where $\tilde{\varepsilon}^*$ is the tensor form of the effective-dielectric constant and $\tilde{I}$ an identity tensor. Eq. (5) is equivalent to the Maxwell equation of Eq. (1), under the $\mathbf{k}\bullet\mathbf{p}$ theory.

三、結果與討論

On the air band, let us consider the temporal evolution of $F(\mathbf{r}, t)$ for an effective isotropic medium. The effective-dielectric tensor becomes a scalar constant ε^*. We shall define the effective speed of the light $c^*=\frac{c}{\sqrt{\varepsilon^*}}$ and the rest mass $\mu=\frac{\hbar\omega_n(q_0)}{c^2}\varepsilon^*$. Eq. (5) can be rewritten as

$$[\frac{\hbar^2}{c*^2}\frac{\partial^2}{\partial t^2}-\hbar^2\nabla^2+(\frac{\hbar\omega_n(q_0)}{c*})^2]F_n(r,t)=0, \quad (6)$$

which is just the Klein-Gordon equation [7] in the relativistic field theory. The Klein-Gordon field can describe particles with the rest mass μ of spin 0. Under the $\mathbf{k}\bullet\mathbf{p}$ theory, we obtain a theory of EM waves propagating in the photonic crystal. This EM wave is a massive field with mass μ. Mass μ is converted from part of the total energy of the EM wave according to the Einstein relation $\varepsilon=mc^2$. The transverse modes and longitudinal mode of EM waves in photonic crystal are coupled, according to the Proca theory of spin 1 massive vector field [8].

Electrons are massive, and so the underlying dispersion relation for electrons in crystals is parabolic. Photons have no mass in the uniform medium, so the underlying dispersion relation is linear. But as a result of the periodicity the photons develop an effective mass in photonic band structure, and this should come as little surprise [9].

By applying the well-known quantization prescription momentum $\mathbf{p}=-i\hbar\nabla$ and energy $E=i\hbar\frac{\partial}{\partial t}$, we obtain from Eq. (6) the relativistic relation between energy and momentum for a free particle of rest mass μ

$$E^2=\mu^2c*^4+p^2c*^2. \quad (7)$$

Eq. (7) shows that the envelope function of EM waves behaves like a free relativistic particle of rest mass μ with momentum $\mathbf{p}$. To study the propagating EM waves in photonic crystals, we shall consider the relativistic effect, which is consistent with the Maxwell equations where the special theory of relativity is satisfied.

If the relativistic effect is negligible, the envelope function of EM waves behaves like a classical particle with slow motion as compared with c*. It then follows that the Klein-Gordon equation becomes the Schrödinger equation in the non-relativistic limit. Under certain conditions, we then have a quantum theory of EM waves propagating in photonic crystals, where no Planck constant $\hbar$ exists.

It is interesting to note that when ε* is negative in the dielectric band, the effective mass would become negative which is certainly invalid. Thus, we have to introduce a concept of "charge" to analogize with electron and hole in semiconductor. The photonic band structure is similar to the conduction and valence bands in semiconductor.

Using the $\mathbf{k}\bullet\mathbf{p}$ theory, we have derived the Klein-Gordon equation to describe the EM wave propagating in photonic crystals. We find that the EM field posses an effective mass which is the photon energy at specific $\mathbf{k}_0$ point divided by square of the effective speed of light c*. The EM field is a massive vector field in photonic crystals. The transverse and longitudinal modes of a massive vector field are coupled. The transverse theory, based on the assumption that the EM wave is a transverse wave, may lose its generality for studying the propagation of EM waves within photonic crystals.

The EM wave is now massive. Its total energy satisfies the relativistic relation between energy and momentum for a free particle. The EM wave propagating in the photonic crystal still posses a relativistic effect only if the speed of light is expressed by c*.

四、計畫成果自評

In our research project, we have developed a theory of EM waves propagating near photonic band gaps. The EM wave is now massive and described by the Klein-Gordon equation. The Klein-Gordon equation is the equation of motion of the spinless particle, which can be charged. Therefore we can first conclude that EM waves propagating near photonic band gaps are massive and charged. But these conclusions are contradicted with our usual belief that EM waves are massless and uncharged. In order not to contradict with our usual sense, we can draw the second conclusion that a new elementary particle is created by EM waves inside the photonic crystal. Either the first conclusion or the second is considering the same story with two opinions. Both conclusions are correct theory of EM waves propagating near photonic band gaps. This discovery shall bring a new horizon for experimentalists to study EM waves propagating near photonic band gaps. We shall be able to study very fundamental problems that how mass, charge and particle can be created by EM waves. We shall send our results to Physical Review for publication.

五、參考文獻

[1] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).

[2] K.M. Ho, C. T. Chan, and C. M. Soukoulis, Phys. Rev. Lett. **65**, 3152 (1990).

[3] K. M. Leung, J. opt. Soc. Am. B **10**, 303 (1993).

[4] J. M. Luttinger and W Kohn, Phys. Rev. **97**, 869 (1955).

[5] N. F. Johnson and P. M. Hui, Phys. Rev. **B48**, 10118 (1993).

[6] J. W. Haus, J. of Modern Optics. **41**, 195 (1994).

[7] O. Klein, Z. Phys. **37**, 895 (1926); W. Gordon, Z. Phys. **40**, 117 and 121 (1926).

[8] C. Itzykson & J. B. Zuber, Quantum Field Theory, McGraw-Hill, 1980.

[9] E. Yablonovitch, J. Opt. Soc. Am. B **10**, 283 (1993).