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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慣性質量的質點運動來描述，若光晶體內具有缺陷存在則此質點會受到缺陷產生之吸引作用而被束縛產生束縛態，質點在空氣能態隙附近的傳遞則缺陷需為介電缺陷方可束縛質點，質點在介電能態隙附近的傳遞則缺陷需為空氣缺陷方可束縛質點，質點束縛能與質點的慣性質量有關，無慣性質量則光晶體內的缺陷無法束縛電磁波。

關鍵詞：慣性質量、束縛態、缺陷

Abstract

Using the $\mathbf{k} \cdot \mathbf{p}$ theory to study photons in a photonic crystal with defects, we found the incident photon excites a quasi-particle (QP) of photon from the periodic background field. This QP contains an inertial mass, which is due to energy-storing mechanism occurring in the photonic crystals. We found that there is an attractive potential which is linear proportional to the product of the inertial mass and the normalized dielectric defect with $V(\mathbf{r}) = -v'(\mathbf{r}) / (1v(\mathbf{r}) + 1v'(\mathbf{r}))$. It is similar to quantum mechanics that the trapping of QP can successfully explain the trapping effect in defects, which cannot be explained by microcavity theory.

Keywords: Defects, Attractive potential, Inertial mass.

二、緣由與目的

Problems of the electromagnetic (EM) wave propagation in multicomponent composites have 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 EM field due to strong interference and diffraction [1]. 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 gap" in analogy with the electronic band gaps in solids. The periodic-dielectric structures are called the photonic-band-gap structures (PBG).

If a small defect is introduced in the photonic crystal, it is possible to create highly localized-defect

modes of the EM wave inside the gap. These defect modes are analogous to the localized impurity states in a semiconductor [3]. To explain how photons are trapped by the defect, the defect is usually treated like a microcavity surrounded by reflecting wall. A microcavity must have a finite volume. But, in one-dimensional crystals, arbitrarily small defects can localize modes [3], which is lack of explanation. In quantum mechanics, there is a phenomenon, like the trapping effect of defects in PBG, that an arbitrarily weak attractive potential can bind a state in one dimensions, but not in three dimensions [4].

From the special relativity, a moving particle with inertial always has a rest frame. However, there is no rest frame for the massless photon, since it moves with the velocity of light c in every frame of reference [5]. It is obvious that a defect can stop and trap a particle with inertial. A defect cannot stop massless photons, but it behaves like a cavity to reflect photons under certain circumstances. Therefore, if a photon in PBG possesses an inertial mass and there is an attractive potential to trap photons, we will explain the trapping effect of defects by proving that the equation of motion of the envelope function indeed includes an inertial mass dependent trap potential.

The appropriate EM equation for studying the photonic crystal is a hermitian equation of magnetic field $\mathbf{H}(\mathbf{r})$:

$$\nabla \times \left[\frac{1}{\epsilon(\mathbf{r})} (1 + V(\mathbf{r})) \nabla \times \mathbf{H}(\mathbf{r}) \right] = \frac{\mathcal{S}^2}{c^2} \mathbf{H}(\mathbf{r}), \quad (1)$$

where $\epsilon(\mathbf{r})$ is the periodic dielectric constant, and assuming $\epsilon'(\mathbf{r})$ is the dielectric constant of defects, the normalized defect dielectric function is then $V(\mathbf{r}) = -\epsilon'(\mathbf{r}) / (\epsilon(\mathbf{r}) + \epsilon'(\mathbf{r}))$. The defect produces a structure perturbation on PBG. We expand $\mathbf{H}(\mathbf{r})$ in terms of Kohn-Luttinger function [6] as $\mathbf{H}(\mathbf{r}) = \sum_{np} A_n(\mathbf{k}) H_{np}(\mathbf{k}, \mathbf{r}) \exp(-i\mathbf{P} \cdot \mathbf{r})$, where

$\mathbf{P} = \mathbf{k} - \mathbf{k}_0$, where \mathbf{k} is a wave vector lies within the first Brillouin zone, and \mathbf{k}_0 is a specific wave-vector in which the band maximum or minimum occurs with $P = |\mathbf{P}| \ll 1$ near the band edge and $A_n(\mathbf{k})$ being the expansion coefficients. $\mathbf{H}_{n,p}(\mathbf{k}, \mathbf{r})$ are the Bloch-type eigenfunctions of Eq.(1) and the corresponding eigenvalues are $\omega_n(\mathbf{k})$, where n is a band index and p represents the index of physical solutions ($\omega_n(\mathbf{k}) \neq 0$) and unphysical solutions ($\omega_n(\mathbf{k}) = 0$). From Notomi's discussions [7], we can define the reciprocal effective-dielectric tensor [8] near the band edge as: [9]

$$\left[\frac{1}{\epsilon^*}\right]_{rs} = \frac{1}{2c^2} \left[\frac{\partial^2 \mathcal{S}_n(\mathbf{k})}{\partial k^r \partial k^s} \right]_{pb} + \frac{1}{2c^2} \left[\frac{\partial^2 \mathcal{S}_n(\mathbf{k})}{\partial k^r \partial k^s} \right]_0 \quad (2)$$

where α and β are indices of three different directions of position vector \mathbf{r} .

三、結果與討論

Following the calculations of de Sterke and Sipe [10] and neglecting defects, $V(\mathbf{r})=0$, we obtain a time-dependent equation of the envelope function $F_n(\mathbf{r},t)$ of Eq. (1) for no defect case:

$$(m_n c)^2 F_n(\mathbf{r}, t) - \left\{ \sum_{rs} \left[\frac{\hbar^2}{\epsilon_n^*} \right]_{rs} \frac{\partial}{\partial x^r} \frac{\partial}{\partial x^s} + \frac{\hbar^2}{c^2} \frac{\partial^2}{\partial t^2} \right\} F_n(\mathbf{r}, t) = 0 \quad (3)$$

This equation is the evolution equation of the EM-wave envelope function under the $\mathbf{k} \cdot \mathbf{p}$ theory, which is the generalized Klein-Gordon equation and is reduced to the Klein-Gordon equation [11] in isotropic medium. This equation indicates there is an energy-storing mechanism near band edges [12], thus we have defined $m_n = \hbar \omega_n(\mathbf{k}_0)/c^2$ as the inertial mass of quasi-particle of photon. The inertial mass m_n is dependent on the band index n and is quantized.

Although, by assuming the band mixing is negligible, we applied the one-band $\mathbf{k} \cdot \mathbf{p}$ theory to study photons near band edges. We can still extend the one-band approximation to the two-band approximation, if the band mixing has to be considered. As long as the incoming radiation was tuned very close to one of band edges, it is still possible to define a single dominating state [10]. Band-mixing effects are just to renormalize the inertial-mass and the effective dielectric tensor. The basic physics of the one-band approximation is unchanged.

Note that the sign of the effective-dielectric tensor derived from the band curvature is positive near the band maximum and negative near the band minimum. Consider the temporal evolution of $F_n(\mathbf{r},t)$ for the positive case of the effective-dielectric tensor and discuss the negative case later. We shall assume that the medium is effectively isotropic. The effective-dielectric tensor becomes a positive scalar constant ϵ^* and the effective speed of the light is $c^* = c/\sqrt{\epsilon^*}$ in the photonic crystal. We can rewrite Eq. (3) as the Klein-Gordon equation:

$$\left\{ \frac{\hbar^2}{c^{*2}} \frac{\partial^2}{\partial t^2} - \hbar^2 \nabla^2 + (\sim_n c^*)^2 \right\} F_n(\mathbf{r}, t) = 0, \quad (4)$$

which has been used to describe a massive spin-zero particle in the relativistic field theory [11] with $\mu_n = m_n \epsilon^*$ being the effective mass of the particle. We

then have a quantum theory of EM waves propagating in PBG, where no Planck constant \hbar exists. The existence of an inertial mass induces the concept of an effective mass in PBG. $\mu_n=0$ in the uniform medium, because there is only one dispersion minimum $\omega_n(\mathbf{k}_0=0)=0$ and $m_n=0$.

By applying the well-known quantization prescription, the momentum operator $\mathbf{P} = -i \hbar \nabla$ and the energy operator $E = i \hbar \frac{\partial}{\partial t}$, to Eq. (4),

we obtain the relativistic energy-momentum relation $E^2 = \mu_n^2 c^{*4} + \mathbf{P}^2 c^{*2}$ for a QP. This relation shows that a Bloch photon behaves as a free relativistic QP moving in a medium with the effective speed of light c^* . The relativistic effect of a free QP is consistent with the Maxwell equations, where the special relativity is satisfied. When the EM wave is entering the photonic crystal, part of the EM-wave energy is stored as the inertial mass m_n of a QP, according to the relation $m_n = \hbar \omega_n(\mathbf{k}_0)/c^2$. The rest part of the EM-wave energy becomes the kinetic energy of a QP, whose velocity \mathbf{v} is not c^* but becomes $\mathbf{v} = \hbar \mathbf{P}/\mu_n$ with $|\mathbf{v}| \ll c^*$, since $P \ll 1$. Therefore EM waves are slowed down near the band edge, which is consistent with observation by Bayindir et al. [13]. When the particle leaves the photonic crystal, the EM wave regains its energy and return to moving velocity of light with no inertial.

If the PBG includes a defect, the formulas governing the behavior of quasi-particles becomes:

$$\frac{(\hbar)^2}{c^2} \frac{\partial^2}{\partial t^2} F_n(\mathbf{r}, t) = [(m_n c)^2 - \sum_{rs} \left[\frac{\hbar^2}{\epsilon_n^*} \right]_{rs} \frac{\partial}{\partial x^r} \frac{\partial}{\partial x^s} + U(\mathbf{r})] F_n(\mathbf{r}, t), \quad (5)$$

where $U(\mathbf{r}) = \pm (m_n c)^2 V(\mathbf{r})$, and + (or -) sign is given for the air-band QP (or the dielectric-band QP). We have neglected a term containing $\nabla V(\mathbf{r})$ in Eq. (5), which is in the order of $P|V(\mathbf{r})|$ and is much less than $|U(\mathbf{r})|$. $U(\mathbf{r})$ is a potential produced by the defect, which produces a perturbation in the space of PBG. $U(\mathbf{r})$ is negative and becomes an attractive potential for the air-band QP, when we add a dielectric defect for $V(\mathbf{r}) < 0$. When we add an air defect for $V(\mathbf{r}) > 0$, $U(\mathbf{r})$ is still an attractive potential for the dielectric-band QP. Dielectric and air defects produce donor and acceptor states, respectively, in the band gap [3]. There is no attractive potential ($U(\mathbf{r})=0$), when the inertial mass of a QP is zero ($m_n=0$). Then, $\nabla V(\mathbf{r})$ has to be considered in Eq. (5) to produce the defect-trapping effect under certain circumstances such as total reflection or reflecting wall for microcavity. Therefore, from the existence of an inertial mass, a QP of Bloch photon can be trapped by an arbitrarily weak attractive potential in one dimension but not in three dimensions [4].

四、計畫成果自評

We have applied the one-band $\mathbf{k} \cdot \mathbf{p}$ theory to study photons in PBG with defects. The incident photon excites a QP from the periodic background field in the crystal. From the energy-storing mechanism occurred in PBG, we find, for the first time, that this QP possesses an inertial. The QP possesses an inertial successfully explains not only the trapping effect of defects analogous to quantum mechanics but also dielectric and air defects produce donor and acceptor states in the PBG. The trapping effect of defects in PBG is similar to that in quantum mechanics, an arbitrarily weak attractive potential can bind a state in one dimension, but not in three dimensions. These phenomena cannot be explained by the microcavity theory that has no attractive trapping potential, when the inertial mass of a QP is zero ($m_n=0$). 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 and why a photon can be trapped by a defect in a photonic crystal. 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] S. Y. Lin *et al.*, Nature (London) **394**, 251 (1998); J. G. Fleming and S.-Y. Lin, Opt. Lett. **24**, 49 (1999).
- [3] E. Yablonovitch *et al.*, Phys. Rev. Lett. **67**, 3380 (1991).
- [4] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1949), see pp. 37 and 77.
- [5] V. B. Berestetskii, E. M. Lifshitz and L. P. Pitaevskii, *Quantum Electrodynamics*, 2nd edition. (Pergamon Press Inc., New York 1979), page 25.
- [6] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).
- [7] M. Notomi, Phys. Rev. B **62**, 10696 (2000).
- [8] N. F. Johnson and P. M. Hui, Phys. Rev. B **48**, 10118 (1993); N. F. Johnson, P. M. Hui and K. H. Luk, Solid State Commun. **90**, 229 (1994).
- [9] J. E. Sipe, Phys. Rev. E **62**, 5672 (2000).
- [10] C. Martijn de Sterke and J. E. Sipe, Phys. Rev. A **39**, 5163 (1999).
- [11] C. Itzykson and J. B. Zuber, *Quantum Field Theory*, (McGraw-Hill Inc., (1980).
- [12] M. Scalora *et al.*, Phys. Rev. E **54**, 1078 (1996).
- [13] Mehmet Bayindir, and E. Ozbay, Phys. Rev. B **62**, 2247 (2000).