Relationship between group velocity and symmetry of photonic crystals

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Group velocity (GV) of eigenmode is a crucial parameter to explain the extraordinary phenomena about light propagation in photonic crystals (PhCs). To study relationships between group velocity and symmetry of PhCs, a new general expression of GV in PhCs made up of non-dispersive material is introduced. Based on this, the GVs of eigenmodes of PhCs, especially those of degenerate eigenmodes at highly symmetric points in the first Brillouin zone, are discussed. Some interesting results are obtained. For example, the summation of degenerate eigenmodes' GVs is invariant under the operations of wave vector $\boldsymbol{K}$-group $M_{\boldsymbol{K}}$. In addition, some numerical results are presented to verify them.

Keywords: group velocity, symmetry, photonic crystals, degenerate eigenmode
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1. Introduction

The transmissions of light in photonic crystals (PhCs) are fascinating issues, because eigenmode of the electromagnetic field in PhCs is a Bloch wave, which is completely different from that in homogeneous materials. Many extraordinary phenomena about light propagation in PhCs are revealed, such as negative refraction,[1−3] super prism phenomenon.[4−6] Group velocity (GV) of eigenmode of PhCs is a crucial parameter to explain these phenomena, because the eigenmode's energy velocity is equal to the group velocity, which is defined as in the expression $\partial\omega/\partial\boldsymbol{K}$. Based on the definition, many approaches have been developed to study GV in PhCs. Such as, the equi-frequency surface(EFS) is used to obtain the direction of GV,[1,2] Feynman–Hellman theorem[7] and $\boldsymbol{K}\cdot\boldsymbol{P}$ perturbation theory[8] are used to calculate the GV in PhCs.

Different from a lot of familiar results about eigenmode's symmetry in PhCs,[7] the relationships between GV and symmetry of PhCs are rarely discussed, especially for the GVs of degenerate eigenmodes. Moreover, the EFS and $\boldsymbol{K}\cdot\boldsymbol{P}$ perturbation theory cannot be directly used to study the relationships between them. So, we introduce a new general expression of the GV based on Feynman–Hellman theorem, which makes theoretical analysis of the GV more convenient.

In Section 2, a general expression of the GV in PhCs is presented. Based on it, the relationships between GV and symmetry of PhCs are discussed in Section 3. In Section 4, some numerical results are shown to verify our results in Section 3. In the paper, we only discuss degenerate eigenmodes caused by the geometrical symmetry.

2. A General expression of GV in PhCs

We generalize the eigen equations of electromagnetic field in PhCs made up of non-dispersive material by the following operator form:

$$\hat{L}(\boldsymbol{X})\circ\boldsymbol{A}_n(\boldsymbol{X})=\lambda_n\boldsymbol{A}_n(\boldsymbol{X})=\frac{\omega_n^2}{c^2}\boldsymbol{A}_n(\boldsymbol{X}). \quad (1)$$

In PhCs, the operator $\hat{L}$ holds for the translational symmetry with lattice vectors $\boldsymbol{R}_n$, that is,

$$\hat{L}(\boldsymbol{X}+\boldsymbol{R}_n)=\hat{L}(\boldsymbol{X}).$$

According to Bloch theorem, the eigenvector of operator $\hat{L}$ can be written as

$$\boldsymbol{A}_{\boldsymbol{K},n}(\boldsymbol{X})=\mathrm{e}^{\mathrm{i}\,\boldsymbol{K}\cdot\boldsymbol{X}}\boldsymbol{u}_{\boldsymbol{K},n}(\boldsymbol{X}), \quad (2)$$

where $\boldsymbol{K}$ is a Bloch vector in the first Brillouin zone (1BZ), $\boldsymbol{u}_{\boldsymbol{K},n}(\boldsymbol{X})$ holds for the same translational symmetry as operator $\hat{L}$ and satisfies

$$\boldsymbol{u}_{\boldsymbol{K},n}(\boldsymbol{X}+\boldsymbol{R}_n)=\boldsymbol{u}_{\boldsymbol{K},n}(\boldsymbol{X}). \quad (3)$$

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By introducing an operator $\hat{L}_{\boldsymbol{K}}$, eigen equation (1) can be reformed into

$$\begin{aligned}\hat{L}_{\boldsymbol{K}} \circ \boldsymbol{u}_{\boldsymbol{K},n} &\equiv \mathrm{e}^{-\mathrm{i}\,\boldsymbol{K}\cdot\boldsymbol{X}}\hat{L}\mathrm{e}^{\mathrm{i}\,\boldsymbol{K}\cdot\boldsymbol{X}} \circ \boldsymbol{u}_{\boldsymbol{K},n} \\ &= \lambda_{\boldsymbol{K},n}\boldsymbol{u}_{\boldsymbol{K},n} = \omega^2_{\boldsymbol{K},n}/c^2\boldsymbol{u}_{\boldsymbol{K},n}. \end{aligned} \quad (4)$$

From Eq. (4), we can prove a new general expression of the GV in PhCs.

Proposition 1 If the operator $\hat{L}_{\boldsymbol{K}}$ in Eq.(4) is an Hermitian operator in the space of periodic field $\Lambda = \{\boldsymbol{v}(\boldsymbol{X}) : \boldsymbol{v}(\boldsymbol{X}+\boldsymbol{R}_n) = \boldsymbol{v}(\boldsymbol{X}), \forall \boldsymbol{R}_n\}$, for an arbitrary vector $\boldsymbol{e}_\alpha$, the GV of eigenmode can be written as

$$\begin{aligned} V_{g(\boldsymbol{K},n)\alpha} &\equiv \boldsymbol{V}_{g(\boldsymbol{K},n)} \cdot \boldsymbol{e}_\alpha \equiv \frac{\partial \omega_{\boldsymbol{K},n}}{\partial \boldsymbol{K}} \cdot \boldsymbol{e}_\alpha \\ &= \frac{c^2}{2\omega_{\boldsymbol{K},n}} \frac{\left\langle \boldsymbol{u}_{\boldsymbol{K},n} \,\middle|\, -\mathrm{i}\left[\boldsymbol{X}\cdot\boldsymbol{e}_\alpha, \hat{L}_{\boldsymbol{K}}\right] \circ \boldsymbol{u}_{\boldsymbol{K},n}\right\rangle}{\langle \boldsymbol{u}_{\boldsymbol{K},n} \mid \boldsymbol{u}_{\boldsymbol{K},n}\rangle} \\ &= \frac{c^2}{2\omega_{\boldsymbol{K},n}} \frac{\left\langle \boldsymbol{A}_{\boldsymbol{K},n} \,\middle|\, -\mathrm{i}\left[\boldsymbol{X}\cdot\boldsymbol{e}_\alpha, \hat{L}\right] \circ \boldsymbol{A}_{\boldsymbol{K},n}\right\rangle}{\langle \boldsymbol{A}_{\boldsymbol{K},n} \mid \boldsymbol{A}_{\boldsymbol{K},n}\rangle}, \end{aligned} \quad (5)$$

where, $\langle \cdots \mid \cdots \rangle$ denotes the inner product, the commutator is defined as

$$\left[\boldsymbol{X}\cdot\boldsymbol{e}_\alpha, \hat{L}_{\boldsymbol{K}}\right] \equiv (\boldsymbol{X}\cdot\boldsymbol{e}_\alpha)\,\hat{L}_{\boldsymbol{K}} - \hat{L}_{\boldsymbol{K}}\,(\boldsymbol{X}\cdot\boldsymbol{e}_\alpha). \quad (6)$$

Proof Differentiating both sides of eigen equation (4) by the component of Bloch vector $K_\alpha = \boldsymbol{K}\cdot\boldsymbol{e}_\alpha$, we have

$$\begin{aligned} &\left[-\mathrm{i}\,\boldsymbol{X}\cdot\boldsymbol{e}_\alpha, \hat{L}_{\boldsymbol{K}}\right] \circ \boldsymbol{u}_{\boldsymbol{K},n} + \hat{L}_{\boldsymbol{K}} \circ \frac{\partial \boldsymbol{u}_{\boldsymbol{K},n}}{\partial K_\alpha} \\ &= \frac{\partial \lambda_{\boldsymbol{K},n}}{\partial K_\alpha}\boldsymbol{u}_{\boldsymbol{K},n} + \lambda_{\boldsymbol{K},n}\frac{\partial \boldsymbol{u}_{\boldsymbol{K},n}}{\partial K_\alpha}. \end{aligned} \quad (7)$$

Since the eigenvector $\boldsymbol{u}_{\boldsymbol{K},n}$ satisfies Eq. (3) and belongs to the set of periodic field Λ, the operator $\hat{L}_{\boldsymbol{K}}$ is an Hermitian operator for $\boldsymbol{u}_{\boldsymbol{K},n}$ and the eigenvalue $\lambda_{\boldsymbol{K},n}$ is real. So, left multiplying both sides of Eq. (7) by $\boldsymbol{u}^*_{\boldsymbol{K},n}$ and integrating over the unit cell of PhCs, we obtain

$$\begin{aligned} \frac{\partial \lambda_{\boldsymbol{K},n}}{\partial \boldsymbol{K}} \cdot \boldsymbol{e}_\alpha &\equiv \frac{\partial \lambda_{\boldsymbol{K},n}}{\partial K_\alpha} \\ &= \frac{\left\langle \boldsymbol{u}_{\boldsymbol{K},n} \,\middle|\, -\mathrm{i}\left[\boldsymbol{X}\cdot\boldsymbol{e}_\alpha, \hat{L}_{\boldsymbol{K}}\right] \circ \boldsymbol{u}_{\boldsymbol{K},n}\right\rangle}{\langle \boldsymbol{u}_{\boldsymbol{K},n} \mid \boldsymbol{u}_{\boldsymbol{K},n}\rangle} \\ &= \frac{\left\langle \boldsymbol{A}_{\boldsymbol{K},n} \,\middle|\, -\mathrm{i}\left[\boldsymbol{X}\cdot\boldsymbol{e}_\alpha, \hat{L}_{\boldsymbol{K}}\right] \circ \boldsymbol{A}_{\boldsymbol{K},n}\right\rangle}{\langle \boldsymbol{A}_{\boldsymbol{K},n} \mid \boldsymbol{A}_{\boldsymbol{K},n}\rangle}, \end{aligned}$$

where the standard notation of "bra" and "ket" vectors have been used, and $\langle \cdots \mid \cdots \rangle$ denotes the inner product, that is,

$$\langle \boldsymbol{u}_{\boldsymbol{K},n} | \boldsymbol{u}_{\boldsymbol{K},n} \rangle \equiv \int_{\text{cell}} \mathrm{d}\boldsymbol{X}\, \boldsymbol{u}^*_{\boldsymbol{K},n}(\boldsymbol{X}) \cdot \boldsymbol{u}_{\boldsymbol{K},n}(\boldsymbol{X}).$$

3. Relationships between GV and symmetry of PhCs

From the symmetries of dispersion curves and eigenmodes in PhCs[7] it follows that if point group G keeps PhCs invariant and its subgroup $M_{\boldsymbol{K}}$ keeps Bloch vector $\boldsymbol{K}$ invariant, then eigenvalues and eigenvectors of $\hat{L}$ in Eq. (1) can be classified according to the irreducible representation (IRREPS) of group $M_{\boldsymbol{K}}$, that is, they can be written as $\lambda^{(l,p)}_{\boldsymbol{K},n}$ and $\boldsymbol{A}^{(l,p)}_{\boldsymbol{K},n}$. In these expressions, l denotes the lth IRREPS, p represents the pth degenerate eigenvector and ranges from one to d_l, the dimension of the lth IRREPS. Giving n and l, the linear space $\Lambda^{(l)}_{\boldsymbol{K},n} = \left\{\boldsymbol{A}^{(l,1)}_{\boldsymbol{K},n}, \boldsymbol{A}^{(l,2)}_{\boldsymbol{K},n}, \ldots, \boldsymbol{A}^{(l,d_l)}_{\boldsymbol{K},n}\right\}$ is a representation space of group $M_{\boldsymbol{K}}$. When a point group operation belonging to group $M_{\boldsymbol{K}}$ is applied to it, all the basis $\boldsymbol{A}^{(l,p)}_{\boldsymbol{K},n}$ of space $\Lambda^{(l)}_{\boldsymbol{K},n}$ transform according the lth IRREPS of group $M_{\boldsymbol{K}}$. Considering the group $M_{\boldsymbol{K}}$ and using Eq. (5), the GV of normalized eigenmodes can be rewritten as

$$\begin{aligned} V^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)\alpha} &\equiv \boldsymbol{V}^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)} \cdot \boldsymbol{e}_\alpha \\ &= \frac{c^2}{2\omega^{(l)}_{\boldsymbol{K},n}} \left\langle \boldsymbol{A}^{(l,p)}_{\boldsymbol{K},n} \,\middle|\, \frac{1}{\mathrm{i}}\left[\boldsymbol{X}\cdot\boldsymbol{e}_\alpha, \hat{L}\right] \circ \boldsymbol{A}^{(l,p)}_{\boldsymbol{K},n}\right\rangle. \end{aligned} \quad (8)$$

Now, we focus on relationship between GV and symmetry of PhCs. Assume spatial point operation $\hat{\Re}$ to belong to point group G, its matrix representation $\boldsymbol{R}$ in the coordinate space will be a real orthogonal matrix and defined as

$$\begin{aligned} &\hat{\Re} \circ \boldsymbol{X} = \boldsymbol{R}_{ij}X_j\boldsymbol{e}_i, \quad \hat{\Re} \circ \boldsymbol{K} = \Re_{ij}K_j\boldsymbol{e}_i, \\ &\boldsymbol{R}^{-1} = \boldsymbol{R}^{\mathrm{T}}, \quad \boldsymbol{R} = \boldsymbol{R}^*. \end{aligned} \quad (9)$$

Since $\hat{\Re}$ keeps PhCs invariant, the operator $\hat{L}$ and this eigenvectors defined as in Eq. (1) must satisfy

$$\begin{aligned} &\hat{\Re} \circ \hat{L} \circ \hat{\Re}^{-1} = \hat{L}, \quad \omega_{\boldsymbol{K},n} = \omega_{\hat{\Re}\circ\boldsymbol{K},n}, \\ &\boldsymbol{A}^{(l,p)}_{\hat{\Re}\circ\boldsymbol{K},n} = \hat{\Re} \circ \boldsymbol{A}^{(l,p)}_{\boldsymbol{K},n}, \quad \forall \Re \in G. \end{aligned} \quad (10)$$

Furthermore, if the operation $\hat{\Re}$ belongs to point group $M_{\boldsymbol{K}}$, that is,

$$\begin{aligned} &\hat{\Re} \circ \boldsymbol{K} = \boldsymbol{K} + \boldsymbol{G}_q, \quad \hat{\Re} \circ \hat{L} \circ \hat{\Re}^{-1} = \hat{L}, \\ &\forall \Re \in M_{\boldsymbol{K}} \in G, \end{aligned} \quad (11)$$

then eigenvectors in Eq. (1) satisfy

$$\begin{aligned} &\hat{\Re} \circ \boldsymbol{A}^{(l,p)}_{\boldsymbol{K},n} = U^{(l)}_{mp}(\Re)\boldsymbol{A}^{(l,m)}_{\boldsymbol{K},n}, \quad U^{(l)}(\Re)^{-1} = U^{(l)}(\Re)^+, \\ &\forall \Re \in M_{\boldsymbol{K}} \in G, \end{aligned} \quad (12)$$

where $\boldsymbol{G}_q$ is an arbitrary reciprocal vector of the PhCs, and the unitary matrixes $\boldsymbol{U}^{(l)}$ is the lth IRREPS matrix of group $M_{\boldsymbol{K}}$.

According to the general expression of GV in PhCs given by Eq. (8) and the symmetries of dispersion curves and eigenmodes given by Eq. (10) and Eq. (12), respectively, it is not hard to prove the following relationships between GV and symmetry of PhCs.

Proposition 2 If point group G keeps PhCs invariant and its subgroup $M_{\boldsymbol{K}}$ keeps Bloch vector $\boldsymbol{K}$ invariant, then the GV of normalized eigenmode in PhCs satisfies

$$\boldsymbol{V}^{(l,p)}_{\mathrm{g}(\hat{\Re}\circ\boldsymbol{K},n)} = \hat{\Re}\circ\boldsymbol{V}^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)} = \boldsymbol{R}_{ij}\boldsymbol{V}^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)j}\boldsymbol{e}_i, \quad \forall\Re\in G, \tag{13}$$

$$\sum_{p=1}^{d_l}\boldsymbol{V}^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)} = \hat{\Re}\circ\sum_{p=1}^{d_l}\boldsymbol{V}^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)} = \sum_{p=1}^{d_l}\boldsymbol{R}_{ij}V^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)j}\boldsymbol{e}_i, \quad \forall\Re\in M_{\boldsymbol{K}}\in G. \tag{14}$$

Proof According to the definitions of a physical field and a spatial point operation, an arbitrary spatial operation $\hat{\Re}$ acting on eigenvectors keeps the inner product in Eq. (8) invariant. So, the following equation can be obtain from Eq. (8):

$$\boldsymbol{V}^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)}\cdot\boldsymbol{e}_\alpha = \frac{c^2}{2\omega^{(l)}_{\boldsymbol{K},n}}\left\langle\hat{\Re}\circ\boldsymbol{A}^{(l,p)}_{\boldsymbol{K},n}\;\middle|\;\hat{\Re}\circ\left(\frac{1}{\mathrm{i}}\left[\boldsymbol{X}\cdot\boldsymbol{e}_\alpha,\hat{L}\right]\;\circ\boldsymbol{A}^{(l,p)}_{\boldsymbol{K},n}\right)\right\rangle. \tag{15}$$

Considering that the symmetry operation $\hat{\Re}$ belongs to point group G, which holds for Eq. (10), Eq. (15) can be rewritten as

$$\boldsymbol{V}^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)}\cdot\boldsymbol{e}_\alpha = \frac{c^2}{2\omega^{(l)}_{\hat{\Re}\circ\boldsymbol{K},n}}\left\langle\boldsymbol{A}^{(l,p)}_{\hat{\Re}\circ\boldsymbol{K},n}\;\middle|\;\frac{1}{\mathrm{i}}\left[\boldsymbol{X}\cdot\left(\hat{\Re}\circ\boldsymbol{e}_\alpha\right),\hat{L}\right]\circ\left(\boldsymbol{A}^{(l,p)}_{\hat{\Re}\circ\boldsymbol{K},n}\right)\right\rangle, \quad \forall\Re\in G. \tag{16}$$

According to the expression of GV defined as in Eq. (8), Eq. (16) means that for an arbitrary vector $\boldsymbol{e}_\alpha$, the GV in PhCs satisfies

$$\boldsymbol{V}^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)}\cdot\boldsymbol{e}_\alpha = \boldsymbol{V}^{(l,p)}_{\mathrm{e}(\hat{\Re}\circ\boldsymbol{K},n)}\cdot\left(\hat{\Re}\circ\boldsymbol{e}_\alpha\right) = \left(\hat{\Re}^{-1}\circ\boldsymbol{V}^{(l,p)}_{\mathrm{e}(\hat{\Re}\circ\boldsymbol{K},n)}\right)\cdot\boldsymbol{e}_\alpha, \quad \forall\Re\in G. \tag{17}$$

Furthermore, considering symmetry operation $\hat{\Re}$ belonging to point group $M_{\boldsymbol{K}}$, from Eqs.(12) and (15), we obtain

$$\boldsymbol{V}^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)}\cdot\boldsymbol{e}_\alpha = \frac{c^2}{2\omega^{(l)}_{\boldsymbol{K},n}}\sum_{m,q}U^{(l)*}_{mp}(\Re)U^{(l)}_{qp}(\Re)\left\langle\boldsymbol{A}^{(l,m)}_{\boldsymbol{K},n}\;\middle|\;\frac{1}{\mathrm{i}}\left[\boldsymbol{X}\cdot\left(\hat{\Re}\circ\boldsymbol{e}_\alpha\right),\hat{L}\right]\circ\boldsymbol{A}^{(l,q)}_{\boldsymbol{K},n}\right\rangle, \quad \forall\Re\in M_{\boldsymbol{K}}. \tag{18}$$

Because $U^{(l)}$ are unitary matrixes, summing both sides of Eq. (18) over index p leads to the following relation of the GV for an arbitrary vector $\boldsymbol{e}_\alpha$:

$$\sum_{p=1}^{m_l}\boldsymbol{V}^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)}\cdot\boldsymbol{e}_\alpha = \sum_{p=1}^{m_l}\boldsymbol{V}^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)}\cdot(\hat{\Re}\circ\boldsymbol{e}_\alpha) = \left(\hat{\Re}^{-1}\circ\sum_{p=1}^{d_l}\boldsymbol{V}^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)}\right)\cdot\boldsymbol{e}_\alpha, \quad \forall\Re\in M_{\boldsymbol{K}}. \tag{19}$$

Proposition 2 means that for a giving Bloch vector $\boldsymbol{K}$, the summation of the GVs of all degenerate eigenmodes in PhCs is invariant under the operation of wave vector $\boldsymbol{K}$-group $M_{\boldsymbol{K}}$. Considering the rotation and the mirror reflection to be two basic spatial point group operations, we can prove two useful results about the GV in PhCs from Proposition 2.

Proposition 3 If a rotational symmetric group $C_m(\boldsymbol{e}_r)$, where positive integer m is larger than one and $\boldsymbol{e}_r$ denotes the direction of rotational axis, is a subgroup of Bloch vector $\boldsymbol{K}$-group $M_{\boldsymbol{K}}$, the summation of the GVs of the degenerate eigenmodes is parallel to the rotational axis, that is,

$$\sum_{p=1}^{d_l}\boldsymbol{V}^{(l,p)}_{\mathrm{g(K,n)}^{(l,p)}} = \left|\sum_{p=1}^{d_l}\boldsymbol{V}^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)}\right|\boldsymbol{e}_r, \quad \forall C_m(\boldsymbol{e}_r)\in M_{\boldsymbol{K}}. \tag{20}$$

Furthermore, if the Bloch vector $\boldsymbol{K}$ is parallel to the rotational axis, the GVs of all eigenmodes are parallel to the rotational axis, that is,

$$\boldsymbol{V}^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)} = \left|\boldsymbol{V}^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)}\right| \boldsymbol{e}_r,$$
$$\forall C_m(\boldsymbol{e}_r) \in M_{\boldsymbol{K}} \in G \ \text{ and } \ \boldsymbol{K}//\boldsymbol{e}_r. \qquad (21)$$

Especially, for two-dimensional (2D) PhCs, the GVs of all eigenmodes at highly symmetric point $\Gamma(0,0)$ are equal to zero, that is,

$$\boldsymbol{V}^{(l,p)}_{\mathrm{g}(\Gamma,n)} = 0, \quad \forall C_m(\boldsymbol{e}_z) \in G. \qquad (22)$$

Proof Because the rotational symmetric group $C_m(\boldsymbol{e}_r)$ is one subgroup of group $M_{\boldsymbol{K}}$, for an arbitrary $\boldsymbol{e}_\alpha$ and an arbitrary spatial rotational operation $\hat{C}^j_m(\boldsymbol{e}_r)$, we can obtain the following equation from Eq. (14):

$$\begin{aligned} m\sum_{p=1}^{d_l} V^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)\alpha} &= \sum_{j=1}^{m}\sum_{p=1}^{d_l} \boldsymbol{V}^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)} \cdot \boldsymbol{e}_\alpha \\ &= \sum_{p=1}^{d_l} \boldsymbol{V}^{(l,p)}_{\mathrm{e}(\boldsymbol{K},n)} \cdot (\sum_{j=1}^{m} \hat{C}^j_m \circ \boldsymbol{e}_\alpha), \\ &\forall \hat{C}^j_m \in M_{\boldsymbol{K}}. \end{aligned} \qquad (23)$$

If the vector $\boldsymbol{e}_\alpha$ is perpendicular to a rotational axis, $\boldsymbol{e}_r$, it is obvious that

$$\sum_{j=1}^{m} \left(\hat{C}^j_m \circ \boldsymbol{e}_\alpha\right) = 0, \quad \forall \boldsymbol{e}_\alpha \cdot \boldsymbol{e}_r = 0. \qquad (24)$$

Combining Eq. (22) and Eq. (23), we can obtain Eq. (20).

Using the same method, Eqs. (21) and (22) can be proven from Eq. (13) in Proposition 2. For 2D PhCs, if there are degenerate eigenmodes at the highly symmetric point $\boldsymbol{K}$, there must be a rotational symmetric group among the subgroups of group $M_{\boldsymbol{K}}$. So, according to Eq. (20) in Proposition 3, at highly symmetric point $\boldsymbol{K}$, the GVs of non-degenerate eigenmode are equal to zero, and the summation of the GVs of two doubly degenerate eigenmodes is equal to zero.

As to a mirror reflection, we can directly obtain the following proposition from Proposition 2.

Proposition 4 If a mirror reflection $\sigma(\boldsymbol{e}_{\boldsymbol{K}\perp})$ belongs to a Bloch vector $\boldsymbol{K}$-group $M_{\boldsymbol{K}}$, where vector $\boldsymbol{e}_{\boldsymbol{K}\perp}$ is the normal vector of the reflection plane and not necessary to be perpendicular to the Bloch vector $\boldsymbol{K}$, the summation of the GVs of the degenerate eigenmodes is parallel to the reflection plane, that is,

$$\sum_{p=1}^{d_l} \boldsymbol{V}^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)} \cdot \boldsymbol{e}_{\boldsymbol{K}\perp} = 0, \quad \forall \sigma(\boldsymbol{e}_{\boldsymbol{K}\perp}) \in M_{\boldsymbol{K}}. \qquad (25)$$

Furthermore, for the Bloch vector $\boldsymbol{K}$ which is parallel to the reflection plane, the GVs of all eigenmodes are parallel to the reflection plane, that is,

$$\boldsymbol{V}^{(l,p)}_{\mathrm{g}(\boldsymbol{K},n)} \cdot \boldsymbol{e}_{\boldsymbol{K}\perp} = 0,$$
$$\forall \sigma(\boldsymbol{e}_{\boldsymbol{K}\perp}) \in M_{\boldsymbol{K}} \in G \ \text{ and } \ \sigma(\boldsymbol{e}_{\boldsymbol{K}\perp}) \circ \boldsymbol{K} = \boldsymbol{K}. \qquad (26)$$

From Proposition 4, we have the following conclusions for 2D PhCs. If there are two mirror reflections $\sigma(\boldsymbol{e}_{\boldsymbol{K}\perp 1})$ and $\sigma(\boldsymbol{e}_{\boldsymbol{K}\perp 2})$, which belong to Bloch ector $\boldsymbol{K}$-group $M_{\boldsymbol{K}}$, with vector $\boldsymbol{e}_{\boldsymbol{K}\perp 1}$ being not perpendicular to vector $\boldsymbol{e}_{\boldsymbol{K}\perp 2}$, the GVs of non-degenerate eigenmodes and the summation of the GV of the doubly-degenerate eigenmodes at $\boldsymbol{K}$ are equal to zero. But, the same condition does not guarantee that the GV of degenerate eigenmode is equal to zero. However, with only the symmetry of dispersion curves about the two mirror planes considered, it is easy to mistake the GVs of all eigenmodes to be equal to zero from the GV expression $\partial\omega/\partial\boldsymbol{K}$. So, Eq. (14) in proposition 2 cannot be obtained directly from the definition of the GV.

4. Numerical results

To verify the propositions about relationships between GV and symmetry of PhCs in Section 3, we calculate the GV of eigenmodes in 2D PhCs by using the plane-wave expansion method and Feynman–Hellman theorem.[7]

The 2D PhCs is a triangular array of cylindrical holes drilled in a dielectric substrate with a relative dielectric constant of 13, and the radii of air holes are all equal to 0.465 (in units of lattice constant a). The band structures and the GVs of TM eigenmodes with Bloch vector $\boldsymbol{K}$ along the ΓK direction are shown in Fig. 1. The left-hand side of Fig.1 shows the band structures calculated by plane-wave expansion method, and the right-hand side of Fig. 1 displays the GVs of eigenmodes obtained from the Feynman–Hellman theorem, where the '$\times$' denotes the component of GV parallel to ΓK (parallel component), and the '$\cdot$' denotes the component perpendicular to ΓK (perpendicular component).

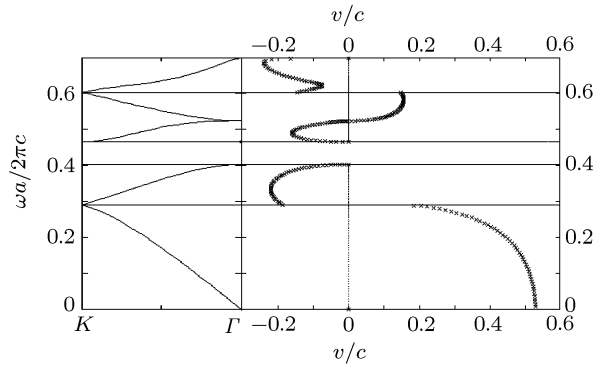


Fig. 1. Band structures (left) and GVs of a PhCs (right) composed of a triangular array of cylindrical holes drilled in a dielectric substrate, where '×' denotes the parallel component and '·' denotes the perpendicular component.

It is obvious that the perpendicular component of the GV on the right-hand side of Fig. 1 is equal to zero. This is consistent with Eq. (26) in our Proposition 4 because the mirror reflection $\sigma(\Gamma K)$ is a symmetrical operation of the PhCs composed of a triangular array of dielectric columns in air. On the other hand, the GVs of eigenmodes at highly symmetric point $\Gamma(0,0)$ are equal to zero. This accords with Eq. (19) in our Proposition 3 in that the $\boldsymbol{K}$-group M_Γ is C_{6V} for the triangular lattices. As to the highly symmetric point K in 1 BZ, the $\boldsymbol{K}$-group M_K is of C_{3V}, which has two singlet and one doublet IRREPSs. So, there must exist a double-degenerate eigenmode at point K. It is not hard to find in Fig. 1 that eigenmodes with normalized frequency equal to 0.29 and 0.60 are two double-degenerate modes. The summation of GVs of these two double-degenerate modes is equal to zero. This is consistent with our Proposition 3, because $C_3(\boldsymbol{e}_z)$ is one subgroup of group $M_{\boldsymbol{K}}$. Moreover, there are two mirror reflections which belong to group $M_{\boldsymbol{K}}$. The normal of one reflection plane is parallel to ΓM, the other is perpendicular to ΓK. The right-hand side of Fig. 1 shows that the GVs of double-degenerate modes at highly symmetric point K are not equal to zero. It accords with our Proposition 4.

Figure 2 (a) shows the dependence of normalized frequency on the Bloch vector in the vicinity of high symmetric point K. Figures 2(b) and 2(c) indicate the EFSs with frequencies between the first band and the second band shown in Fig. 1, respectively. It is worth noticing that at the eigenfrequency of one double-degenerate eigenmode, 0.29, the EFS shrinks into an isolated point. So, it is not likely to indicate the direction of the degenerate eigenmode GV from the EFS.

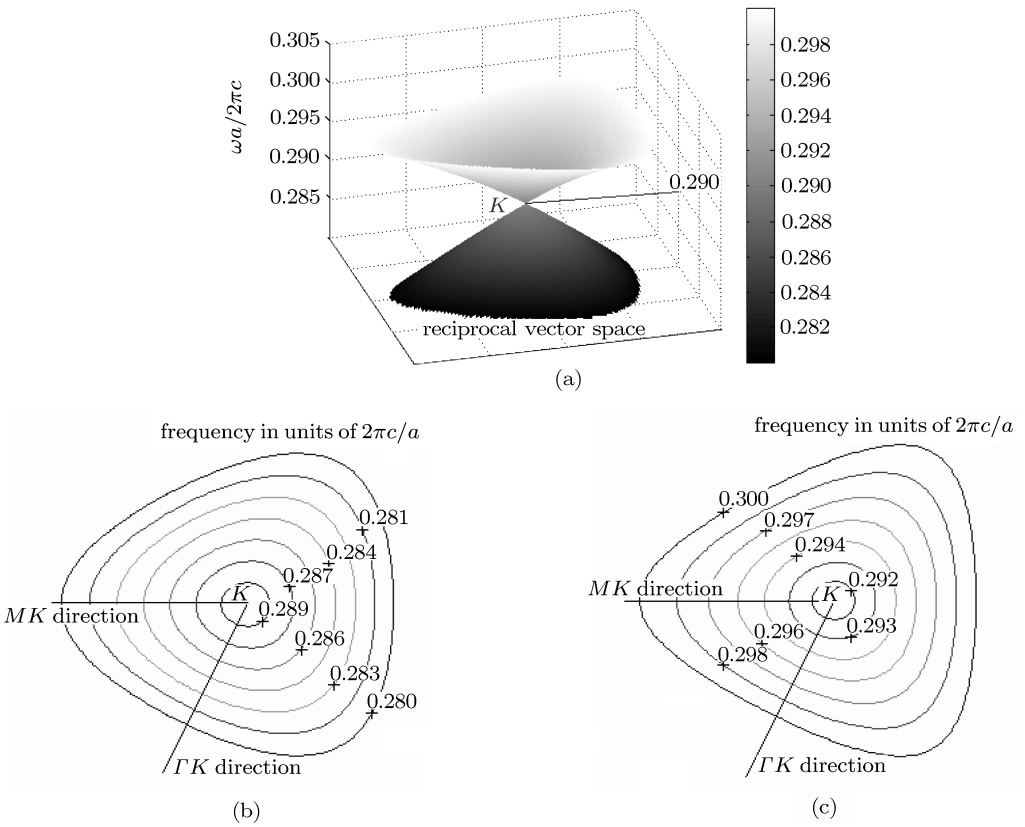


Fig. 2. Dependence of normalized frequency on Bloch vector in the vicinity of high symmetric point K (a), EFSs with frequencies between the first band (b) and the second band (c).

5. Conclusions

To discuss relationships between GV and symmetry of PhCs made up of non-dispersive material, we introduce a general expression of the GV of eigenmode in PhCs. Based on it, we obtain some useful results of the GVs of eigenmodes at highly symmetric points in 1BZ. For example, for a given Bloch vector $\boldsymbol{K}$, the summation of the GVs of all degenerate eigenmodes in PhCs is invariant under the operation of wave vector $\boldsymbol{K}$-group $M_{\boldsymbol{K}}$. Especially, at a rotational symmetric point, the GVs of non-degenerate eigenmodes and the summation of the GVs of the degenerate eigenmodes are parallel to the rotational axis. At a mirror reflection symmetric point, the GVs of non-degenerate eigenmodes and the summation of the GVs of the degenerate eigenmodes are parallel to the reflection plane.

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