Structure-Preserving Methods for Computing Complex Band Structures of Three Dimensional Photonic Crystals [1]

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Abstract This work is devoted to the numerical computation of complex band structure $\mathbf{k} = \mathbf{k}(\omega) \in \mathbb{C}^3$ for positive frequency ω of 3D isotropic dispersive or non-dispersive photonic crystals from the perspective of gyroscopic quadratic eigenvalue problems (GQEPs). Our basic strategy is to fix two degrees of freedom in k and to view the remaining one as the eigenvalue of a quadratic operator pencil derived from Maxwell's equations. Then Yee's scheme is employed to discretize $\nabla\times$and $\boldsymbol{k}\times$ operators in this quadratic operator pencil. Furthermore, we reformulate this QEP into an equivalent T-palindromic QEP (T-PQEP) for which we have established the structure-preserving algorithm, namely, the generalized T-skew-Hamiltonian implicit restarted Arnoldi algorithm (GTSHIRA).

Problem Description The electromagnetic fields in dispersive photonic crystals (PCs) are governed by the following source-free Maxwell's equations (MEQs) in the frequency domain,

(1) $\nabla \times \mathbf{E} = -\imath\omega\mu(\boldsymbol{x},\omega)\mathbf{H}, \quad \nabla \times \mathbf{H} = \imath\omega\varepsilon(\boldsymbol{x},\omega)\mathbf{E},$

where $\mu,\varepsilon\colon \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}$ are the permeability and permittivity of a isotropic dispersive material, which are lattice-periodic with lattice vectors $\{\mathbf{a}_\ell\}_{\ell=1}^3$. Then, from Bloch theorem, $\mathbf{E}$ and $\mathbf{H}$ in (1) can be factorized into $\mathbf{E} = e^{\imath\mathbf{k}\cdot\mathbf{x}}\boldsymbol{E_p}$and $\mathbf{H} = e^{\imath\mathbf{k}\cdot\mathbf{x}}\boldsymbol{H_p}$ where $\mathbf{k} \in \mathbb{R}^3$ denoted the wavevector and $\boldsymbol{E_p}, \boldsymbol{H_p}$ are periodic in conformity with μ and ε. In the case of non-dispersive PCs, usually the wave vector $\mathbf{k} \in \mathbb{R}^3$ is chosen beforehand, and MEQs (1) are discretized into a constrained eigenvalue problems w.r.t ω. By solving a few smallest positive ω's for different $\mathbf{k}$, we obtain the dispersion curves $\omega = \omega(\mathbf{k})$ or the standard band structures (BSs) [2,3]. Due to the nonlinearity of μ or ε on ω, it is more challenging to compute the dispersion curves $\omega = \omega(\mathbf{k})$, as shown in [4]. Moreover, in many cases, μ or ε is a rational function of ω in the partial fraction form with more than two terms, then the rational eigenvalue problem w.r.t. ω is transformed into a polynomial eigenvalue problem with a relatively high degree, which is still not easy to solve. However, it is much more convenient to adopt an opposite perspective that the wave vector $\mathbf{k}$ is viewed as a function $\mathbf{k} = \mathbf{k}(\omega)$ of the real frequency ω. In this case, we only solve the QEP to compute the complex BS $\mathbf{k} = \mathbf{k}(\omega)$, i.e., to solve $\mathbf{k} \in \mathbb{C}^3$ such that $\omega(\mathbf{k})$ is equal to a positive constant.

Main Schema Let $\mathbf{k} = \lambda\tilde{\mathbf{k}}$ with unit vector $\tilde{\mathbf{k}}$ and complex wave number $\lambda \in \mathbb{C}$. Then (1) can be reduced into the following constrained quadratic operator pencil (assumed with $\mu(\boldsymbol{x},\omega) \equiv 1$)

(2) $\left(\iota\lambda\tilde{\mathbf{k}} + \nabla\right) \times \left(\iota\lambda\tilde{\mathbf{k}} + \nabla\right) \times \boldsymbol{E_p} = \omega^2\varepsilon(\boldsymbol{x},\omega)\boldsymbol{E_p}.$

We use Yee's scheme to discretize (2) to yield a GQEP

(3) $(\tau^2 M + \tau G + K)\boldsymbol{e} = \mathbf{0}, \ \tau = \iota\lambda$

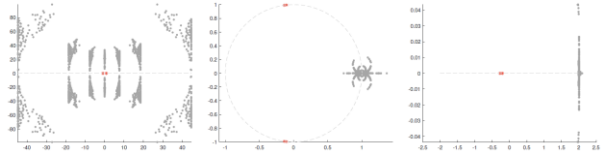
where $M^{\mathrm{T}} = M$, $G^{\mathrm{T}} = -G$, $K^{\mathrm{T}} = K$. Furthermore, under the Cayley transformation, we map the GQEP to a T-PQEP

(4) $\left(\nu^2 A^{\mathrm{T}} - \nu Q + A\right)\boldsymbol{e} = \mathbf{0}, \ \nu = \pm\frac{1+\tau}{1-\tau},$

with $Q^{\mathrm{T}} = Q$. Finally, via the T-symplectic linearization and the $(S + S^{-1})$-transform, the T-PQEP is transformed into a T-skew-Hamiltonian pencil of a T-skew-Hamiltonian pair $(\mathcal{K},\mathcal{N})$ as

(5) $\mathcal{K}\boldsymbol{u} = \eta\mathcal{N}\boldsymbol{u}, \ \eta = \nu + \nu^{-1},$

which we would solved via the GTSHIRA.



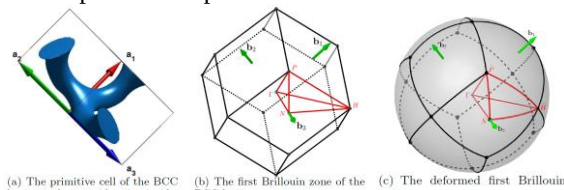
(a) The distribution of λ's with $|\lambda| < 100$. (b) The image of those λ's under $\nu = \nu(\lambda)$. (c) The image of those λ's under $\eta = \eta(\lambda)$.

(Red dots denoted the target wave numbers)

References

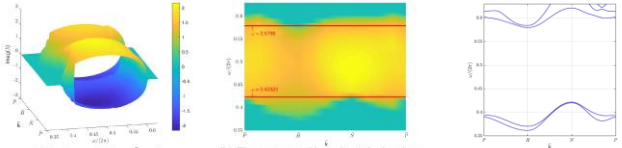
[1]. *Structure-Preserving Methods for Computing Complex Band Structures of Three Dimensional Photonic Crystals*, J. Sci. Comput., to appear (2020).
[2]. *Eigendecomposition of the discrete double-curl operator with application to fast eigensolver for three dimensional photonic crystals*. SIAM J. Matrix Anal. Appl. (2013).
[3]. *Solving three dimensional Maxwell eigenvalue problem with fourteen Bravais lattices.* Tech. rep., arXiv, (2018).
[4]. *Structure-preserving algorithms for palindromic quadratic eigenvalue problems arising from vibration on fast trains*. SIAM J. Matrix Anal. Appl. 30, (2008).

Numerical Experiments We consider the 3D PC with the BCC lattice structure, in its primitive cell there were two different media separated by the interface of a single gyroid structure. The permittivity of the media inside the single gyroid region is $\varepsilon_1(\omega)$, while the rest space of the primitive cell is just air.



(a) The primitive cell of the BCC lattice with a gyroid region inside. (b) The first Brillouin zone of the BCC lattice. (c) The deformed first Brillouin zone.

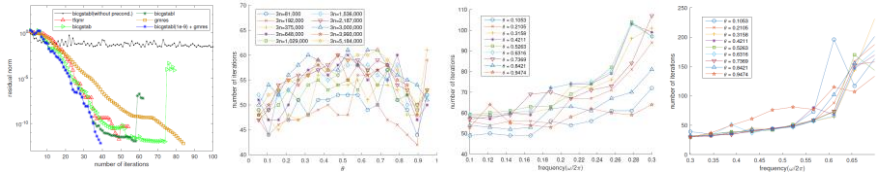
Benchmark Problem: Non-dispersive PC ($\varepsilon_1(\omega) \equiv 16$) By chosen $\omega \in [0.3,0.7]$ and $\tilde{\mathbf{k}}$ over the deformed first Brillouin zone, we can draw the imaginary part of those complex wave numbers which have smallest imaginary parts and compare between the standard BS (ω) and the complex BS (λ).



(a) Surfaces of $\Im\lambda$ *vs.* $\tilde{\mathbf{k}}$ and ω. (b) The estimate of bounds of the bandgap. (d) A snapshot of the standard band structure.

Numerical Efficiency of GTSHIRA on Dispersive PC ($\varepsilon_1(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega-\iota\gamma_p)}$)

In GTSHIRA, we proposed a preconditioned linear system to deal with each iteration, which were get a pretty good performance on various parameters.



Furthermore, the average iteration numbers of GTSHIRA corresponding to each unit wave vectors were quite stable.

Table 1 The average number of restarts (ANR) of GTSHIRA for the non-dispersive model

$\mathbf{k}$	P	$(3P+H)/4$	$(P+H)/2$	$(P+3H)/4$	H	$(3H+N)/4$
ANR	3.7	2.4	2.5	2.8	3.5	2.5
$\mathbf{k}$	$(H+N)/2$	$(H+3N)/4$	$(N+P)/2$	$(3N+P)/4$	N	$(N+3P)/4$
ANR	2.4	2.8	2	2.8	2.3	2