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A Novel Structure-Preserving Algorithm with Green's Function Approach for Computing Band Structures of Photonic Quasicrystals

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Abstract. A novel bi-infinite approach to compute the band structures of 2D photonic superlattices with 1D quasicrystal sequences is devised. Leveraging strategically the bi-infinite characteristic, the approach first transforms the infinite-dimensional eigenvalue problem into a finite-dimensional nonlinear eigenvalue problem (NEVP) on a single cell for efficient numerical solution. Challengingly, the NEVP is built upon the solutions to two systems of cyclic nonlinear matrix equations (NMEs) that have to be solved repeatedly during iteratively solving the NEVP. The solutions are efficiently calculated by a newly developed highly efficient coalescing technique followed by a structure-preserving doubling algorithm. It is showed that the cost of coalescing is proportional to the logarithm of N, the length of the truncated quasicrystal sequence, which is significant as the cost of coalescing becomes more noticeable as N gets bigger for highly accurate simulations. Finally, through mathematical analysis, inclusion intervals for eigenvalue of interest are estimated so as to significantly narrow down the scope of search, and that significantly contributes to the overall efficiency of the approach, as the NEVP is nonlinear in nature and has to be solved iteratively.

AMS subject classifications: 65F15, 65M80, 65M60, 78M10

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1 Introduction

Photonic quasicrystals (PQCs) [4, 23, 30], celebrated for their distinctive aperiodic order and intricate symmetries, have attracted considerable attention owing to their ability to manipulate light in novel ways. These structures present unique opportunities for directing photon flow, potentially advancing optical communication, sensing, and imaging technologies. Computational investigations of PQCs allow researchers to examine their bandgap properties and light propagation features, aiding the development of efficient photonic devices such as waveguides, lasers, and filters [22, 26, 34].

In the field of quasicrystal structure computation, the supercell approximation and projection methods are two of the most widely used techniques. These methods are crucial for simulating the complex aperiodic order inherent in photonic quasicrystals. The supercell approximation [24, 36, 39] constructs a sufficiently large periodic structure that mimics the quasicrystal, thereby enabling the use of traditional computational approaches. On the other hand, the projection method [13, 14, 25] maps low-dimensional photonic quasicrystals into a higher-dimensional periodic lattice, effectively capturing the aperiodic nature of quasicrystals. Both methods, however, require substantial computational resources to achieve high precision, as they must accurately account for complex interference patterns and subtle photonic bandgap effects. Consequently, enhancements in both computational power and algorithmic efficiency are vital for conducting detailed and accurate simulations, which are essential for designing optimally innovative photonic devices.

For approximating an 1D quasi-periodic structure using periodic structures, as shown in Fig. 1a, a supercell is a periodic unit created to contain as many cells as possible so that the quasi-periodic structure of interest is adequately approximated. There are two different ways to do so. One is to simply use a sufficiently large supercell and then repeats it, as in Fig. 1a where one supercell AB$\cdots$BA appears periodically. The other one which we will be using is to first select a central cell C (the *scattering region*) and then create two supercells, one for each sides of the scattering region, as shown in Fig. 1b where the scattering region is in the middle marked by C and to its left is supercell AB$\cdots$BA repeated and to its left is a different supercell AB$\cdots$AA repeated. This introduces an additional flexibility to account for different long-range periodic growths to the two sides of the scattering region, thereby reformulating the original model as an approximate bi-infinite one.

In this study, we focus on the band structure calculations for 2D photonic superlattice (PS) with 1D quasi-periodicity. By leveraging the supercell approximation, we employ a novel cyclic reduction technique to condense the computations involving large supercell structures into a manageable unit cell size. This means that even though a substantial number of supercells are necessary to approximate PS accurately, the actual dimension of the discrete eigenvalue problem remains relatively small when it comes to compute the band structure. This significantly reduces the computational complexity in the overall band structure calculation for 2D photonic superlattice, making it numerically efficient