Step approximation of oblique boundaries to compute band structures of photonic crystals

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We want to determine the band structures of photonic crystals with hexagonal elementary cell. Oblique coordinates had been successfully applied for this purpose (see e.g. [1] [2]). However, when we use the method of lines [3] or finite differences as numerical algorithms we obtain matrices whose size is twice as large as those appearing when Cartesian coordinates are used. If rectangular cells are used instead, the area is twice as large as that of the elementary cell leading to non-unique values of the bands.

Here, we want to combine these approaches, i.e. use oblique boundaries and perform the calculations with Cartesian coordinates. For this purpose, we introduce a step approximation (see Fig. 1a). Now, a step approximation of waveguide structures is commonly used (e.g. for modeling a tilted waveguide) and one might wonder about the novelty. As one can see in Fig. 1a) the boundaries of the computational window itself is modeled with a staircase approximation. This is in contrast to the analysis of tilted waveguides, where the step approximation is only done for the inner structure, whereas the outer boundaries remain homogeneous.

By looking at the point labeled $k$ in Fig. 1a we see the difficulties when we model the computational window with stairs. As known, the wave equation contains derivatives with respect to the vertical (here $z$) coordinate. If we use e.g. finite differences, we need the points $k - 1$ and $k + 1$ for an approximation of these derivatives. If we apply the method of lines [3] as alternative numerical method we divide the structure into homogenous regions. (The two lowest ones are labeled $A$ and $B$ in Fig. 1a). As can be seen, for both cases we must consider the area outside the computational window. Now, for the computation of band structures in PhCs, we know that the fields are periodic in horizontal ($x$ resp. $v$) direction. This permits us to transform the fields from the right boundary to left one.

A second problem is indicated in Fig. 1a as well. The PhC is periodic in $v$ and $u$ direction. However, when using Cartesian coordinates, we relate the point “1” and “2”, whereas we know from the oblique coordinate system that point “1” and point “3”, have to be connected. Mathematically, we solve this problem by introducing a ”virtual layer” at the top boundary, which causes a ”shift” of the fields to relate the correct fields at the top and bottom boundary with each other. Numerical results obtained with oblique coordinates and with a step approximation (Cartesian coordinates) are shown in Fig. 1b. A very good agreement can be recognized.

Fig. 1: a) Elementary cell of a hexagonal photonic crystal and step approximation; b) determined band structure

