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Numerical Simulation of Waves in Periodic Structures

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Abstract. In this work we improve and extend a technique named *recursive doubling procedure* developed by Yuan and Lu [J. Lightwave Technology 25 (2007), 3649-3656] for solving periodic array problems. It turns out that when the periodic array contains an infinite number of periodic cells, our method gives a fast evaluation of the exact boundary Robin-to-Robin mapping if the wave number is complex, or real but in the stop bands. This technique is also used to solve the time-dependent Schrödinger equation in both one and two dimensions, when the periodic potential functions have some local defects.

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1 Introduction

Nowadays periodic structure problems arise quite often in many modern application areas like semiconductor nanostructures (e.g. quantum dots and nanocrystals), semiconductor superlattices [6, 36], photonic crystal (PC) structures [5, 25, 29], meta materials [31] or Bragg gratings of surface plasmon polariton (SPP) waveguides [18, 32].

The most interesting property of these periodic media, especially in optical applications, is the capability to select the ranges of frequencies of the waves that are allowed to pass or blocked in the waveguide ('frequency filter'). Waves in (infinite) periodic media only exist if their frequencies lie inside these allowed continuous bands separated by forbidden gaps. This fact corresponds mathematically to the gap structure of the differential

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operator having so-called *pass bands* and *stop bands*. Numerical simulations are necessary for the design, analysis and finally optimization of the waveguiding periodic structures.

In many cases these wave propagation problems are modeled by periodic partial differential equations (PDEs) on unbounded domains and for solving these equations numerically one has to confine the spatial domain to a bounded computational domain (in a neighborhood of the region of physical interest). *Artificial boundaries* are thus necessary to be introduced and adequate boundary conditions should be imposed. Note that even in the case of a bounded but large domain, it is a common practice to reduce the original domain to a smaller one by introducing artificial boundaries, for example, see [27].

The ideal boundary conditions at the artificial boundaries should not only lead to well-posed problems, but also mimic the perfect absorption of waves leaving the computational domain through the artificial boundaries. Moreover, these boundary conditions should allow for an easy implementation. These boundary conditions are usually called *absorbing* (or transparent, non-reflecting in the same spirit) in the literature. We refer the interested reader to a couple of review papers [3, 14, 16, 17, 35] on this fundamental research topic.

Though *absorbing boundary conditions* (ABCs) for wave-like equations have been a hot research issue for many years and many developments have been made on their designing and implementing, the issue of exact ABCs for periodic structure problems is still not fully-resolved. Some progresses can be found in the recent research articles [9, 10, 12, 13, 23, 30, 33, 34, 38–40] and [42]. For a review on the theory of waves in locally periodic media including a survey on physical applications we refer the reader to [15].

In the existing literature *frequency domain methods* (FDMs) are usually considered for wave problems with periodic structures [22]. These methods are able to exploit the special geometric structure and are based on an eigenmode expansion in every longitudinally uniform cell. Frequently, the FDMs are used in conjunction with the *perfectly matched layer* (PML) [7] technique for dealing with unbounded domains. Afterwards the *bidirectional beam propagation methods* (BiBPMs) [20] were introduced. Like the FDMs, they can utilize the periodic geometry but additionally they (and also the *eigenmode expansion methods* in [7] and [20]) are able to resolve the multiple reflections at the longitudinal interfaces.

The methods of Jacobsen [21] and Yuan & Lu [38] were developed to be more efficient than the eigenmode expansion methods, because it turns out that solving the eigenmodes in each segment is quite time consuming. More recently, a *DtN mapping method* [37] was developed by Yuan and Lu that is more accurate than the BiBPMs, since this approach works (mostly) without any approximation. In [39] the efficiency of this sequential DtN approach was further improved by a *recursive doubling process* for the DtN map.

In this paper we study a numerical method for the *Helmholtz equation*

$$-\Delta u(\mathbf{x}) + Vu(\mathbf{x}) + zn^2 u(\mathbf{x}) = f(\mathbf{x}). \tag{1.1}$$

Here z is a complex parameter, $V = V(\mathbf{x})$ and $n = n(\mathbf{x})$ are two sufficiently smooth real