Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Evaluation of exact boundary mappings for one-dimensional semi-infinite periodic arrays

Matthias Ehrhardt[1], Jiguang Sun[2] , Chunxiong Zheng[3]

submitted: 17th September 2008

[1] Weierstraß Institut für Angewandte Analysis und Stochastik
Mohrenstraße 39, 10117 Berlin, Germany
email: ehrhardt@wias-berlin.de

[2] Applied Mathematics and Theoretical Physics Department
Delaware State University
Dover, DE 19901, USA
email: jsun@desu.edu

[3] Department of Mathematical Sciences, Tsinghua University
Beijing 100084, P.R. China
email: czheng@math.tsinghua.edu.cn

No. 1358
Berlin 2008

2000 *Mathematics Subject Classification.* 65M99 35B27 35Q60, 35J05.

Key words and phrases. periodic arrays, Helmholtz equation, Sommerfeld-to-Sommerfeld mapping, dispersion diagram, Floquet-Bloch theory.

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract. Periodic arrays are structures consisting of geometrically identical subdomains, usually called periodic cells. In this paper, by taking the Helmholtz equation as a model, we consider the defnition and evaluation of the exact boundary mappings for general one-dimensional semi-infnite periodic arrays for any real wavenumber. The well-posedness of the Helmholtz equation is established via the limiting absorption principle.

An algorithm based on the doubling procedure and extrapolation technique is proposed to derive the exact Sommerfeld-to-Sommerfeld boundary mapping. The advantages of this algorithm are the robustness and simplicity of implementation. But it also suffers from the high computational cost and the resonance wave numbers.

To overcome these shortcomings, we propose another algorithm based on a conjecture about the asymptotic behaviour of limiting absorption principle solutions. The price we have to pay is the resolution of two generalized eigenvalue problems, but still the overall computational cost is significantly reduced. Numerical evidences show that this algorithm presents theoretically the same results as the first algorithm. Moreover, some quantitative comparisons between these two algorithms are given.

1. Introduction. These days periodic array problems arise frequently in many up-to-date application areas like photonic crystals (PC) [26], [30], [35], semiconductor nanostructures (e.g. quantum dots and nanocrystals), semiconductor superlattices [4], [50], meta materials [42] or Bragg gratings of surface plasmon polariton (SPP) waveguides [19], [43].

The most interesting property of periodic arrays, especially in optical applications in nano- and micro-technology, is the capability of selecting waves in a range of frequencies that are allowed to pass or blocked through the media. Waves in periodic arrays only exist when their frequency lies inside some allowed continuous bands separated by forbidden gaps. This fact corresponds mathematically to the dispersion diagram of suitable differential operator having so-called *pass bands* and *stop bands.* Since the governing wave equation is either of periodic variable coefficient, or defined on a domain consisting of periodic subregions, theoretical analysis is very limited, and numerical simulation is a fundamental tool for the design, analysis and finally optimization of the periodic arrays.

In many cases some defect cells are artificially introduced into a perfect periodic array for some additional interesting property. For example, if the defect cells are properly designed, some defect modes [41] can exist for certain frequencies in the band gaps. This phenomena has many important applications, e.g. in light emitting devices (LEDs) and photonic circuits [34].

In general, efficient numerical simulations are necessary for the design, analysis and finally optimization of the waveguiding periodic structures. However, in many cases these wave propagation problems are modeled by partial differential equations (PDEs) on very large domains, e.g. the wanted frequencies of these defect modes are the eigenvalues of a PDE eigenvalue problem posed on an *unbounded domain* [17].

For solving these PDEs numerically, a common practice is to confine the real computational domain by introducing *artificial boundaries* to enclose a small neighbourhood of the region with physical interest. Note that even in the case of a bounded domain of a periodic media it is common practice for a numerical simulation with high accuracy to reduce the original spatial domain to some smaller region of interest by introducing artificial boundaries in order to resolve the very fine periodic structures accurately. This is especially beneficial if these generated *exterior domains* consist of a huge number of periodicity cells.

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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 *artificial* (or transparent, non–reflecting, absorbing in the same spirit) in the literature. Basic requirements for *artificial boundary conditions* (ABCs) are well–posedness and easy (relatively) implementation. Furthermore, a fast, efficient and accurate evaluation of the *Dirichlet-to-Robin* (DtR) mapping is essential. We refer the interested reader to a couple of review papers [2, 15, 18, 47] on this fundamental research topic.

Let us remark that ABCs for linear PDEs have been a hot research issue for many years and many developments have been made on the designing and implementing of various ABCs, also for multi–dimensional and nonlinear problems [2]. However, the question of exact ABCs for periodic structure problems is not fully settled yet and is a very current research topic, cf. the recent papers [11], [13], [14], [27], [38], [40], [45], [46], [52], [53], [54]. For a comprehensive review on the theory of waves in locally periodic media including a survey on physical applications we refer the interested reader to [16].

2. A model problem. We consider a closed waveguide consisting of an infinite number of identical cells, see Fig. 2.1. There C_j denotes the j-th periodic cell, and Γ_j the j-th cell boundary. The governing wave equation is the *Helmholtz equation*

$$\Delta u + k^2 n^2 u = 0, \qquad (x,y) \in \Omega = \cup_{j=1}^{+\infty} \mathrm{C}_j, \tag{2.1}$$

where k is the reference wave number, and $n = n(x,y)$ is the refraction index function. On each cell boundary Γ_j we define two *Sommerfeld data* associated with the function u as

$$f_j(u) = (\partial_x + ik)u|_{\Gamma_j}, \qquad g_j(u) = (\partial_x - ik)u|_{\Gamma_j}, \tag{2.2}$$

where i denotes the imaginary unit. To clarify the physical meaning of these two data, let us first return to the one-dimensional constant coefficient Helmholtz equation

$$u_{xx}+k^2u=0.$$

Two linearly independent solutions are $e^{\pm ikx}$. As a common convention, e^{ikx} represents a wave traveling to the right, and e^{-ikx} to the left. An easy computation yields

$$(\partial_x+ik)e^{ikx}=2ike^{ikx}, \qquad (\partial_x-ik)e^{ikx}=0,$$

and

$$(\partial_x+ik)e^{-ikx}=0, \qquad (\partial_x-ik)e^{-ikx}=-2ike^{-ikx}.$$

These expressions above imply that the operator ∂_x+ik eliminates the left-going wave while the operator ∂_x-ik eliminates the right-going wave. Thus, the functions f_j and g_j in (2.2) contain some information about the right-going and left-going waves respectively. They are further referred to as *incoming* or *outgoing* relying on the location of Γ_j with respect to (w.r.t.) the concerned part of the domain. For example, w.r.t. C_j, f_j is incoming and g_j is outgoing, but w.r.t. C_{j-1}, f_j is outgoing and g_j is incoming.

The boundary conditions on the top, bottom and interior (if existing) boundaries could be either Neumann or Dirichlet, or any combination, but they need to be consistent with the geometry periodicity. Moreover, these boundary conditions should guarantee the well–posedness of the Helmholtz equation (2.1) on the union of any finite number of periodic cells, say $\cup_{j=0}^{N-1}\mathrm{C}_j$, if the incoming Sommerfeld data are prescribed on its left and right boundaries, say Γ_0 and Γ_N.

We remark that these restrictions are in fact very mild thanks to the Holmgren uniqueness theorem [23, Section 5.3]. In the sequel, if not specified otherwise, we assume homogeneous Neumann boundary conditions at the top and bottom boundaries.

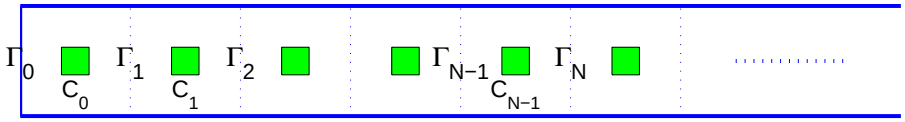

FIG. 2.1. *Schematic view of a semi-infinite periodic array.* C_j *denotes the* j*-th periodic cell.* Γ_j *is the left cell boundary of* C_j *and the right cell boundary of* C_{j-1} *(for* $j\geq 1$*).*

Three different periodic arrays (PA) will be considered in this paper, and we will refer to them as PA-One, PA-Two and PA-Three. All of them consist of periodic cells with size of 1×1. More details are listed in the following list:

- **PA-One**. Homogeneous waveguide. $n=1$.
- **PA-Two**. A hold of size 0.5×0.5 is located in the center of every periodic cell. Zero Dirichlet boundary condition is applied at the hole boundary. $n=1$.
- **PA-Three**. Rectangular waveguide. $n(x,y)=1+0.5\cos(2\pi x)\sin(2\pi y)$.

To explore the wave property in a periodic array, it is usually helpful to consider the dispersion diagram of the characteristic equation $-\Delta u=En^2u$, restricted to a

single periodic cell, say C_0. The boundary conditions at the left and right boundaries are *pseudoperiodic*, namely,

$$u|_{\Gamma_1} = e^{i\theta} u|_{\Gamma_0}, \qquad u_x|_{\Gamma_1} = e^{i\theta} u_x|_{\Gamma_0},$$

where the parameter θ is valued in $[0, 2\pi)$. For each θ, there exists a sequence of real eigenvalues E, usually called *energies*. All energies E w.r.t. θ then compose the dispersion diagram. The dispersion relation for PA-One, the homogeneous waveguide, can be obtained analytically as

$$E_{jm} = j^2\pi^2 + (\theta + 2\pi m)^2.$$

This multi-valued function is plotted in Fig. 2.2. For PA-Two and PA-Three, no analytical expressions of dispersion relation are available, and a spatial discretization method has to be employed. We use the eighth-order FEM method with mesh sizes $\Delta x = \Delta y = 0.125$ for all the numerical tests reported in this paper.

The dispersion diagrams for PA-Two and PA-Three are shown in Figs. 2.3-2.4. A significant phenomena could be observed that unlike the homogeneous waveguide, there are some bands of energy values in the dispersion diagrams of PA-Two and PA-Three that could not be reached for any parameter θ.

Physically, waves with energy (here k^2) in these bands could not propagate in the medium. Right in this context, they are usually referred to as *stop bands* in the literature. In fact, it is exactly this remarkable property which makes the periodic structures extremely useful, for example, they could be elaborately designed to act as some kind of frequency selecting modules in the microwave and optical engineering.

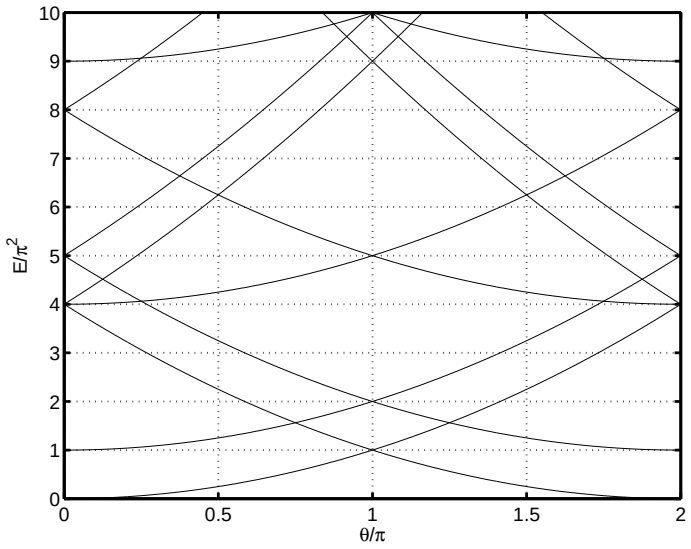

FIG. 2.2. *Dispersion diagram of PA-One, an homogeneous waveguide.*

This work is aimed at developing an efficient method for deriving an exact boundary mapping of semi–infinite periodic arrays for *any real wavenumber* k.

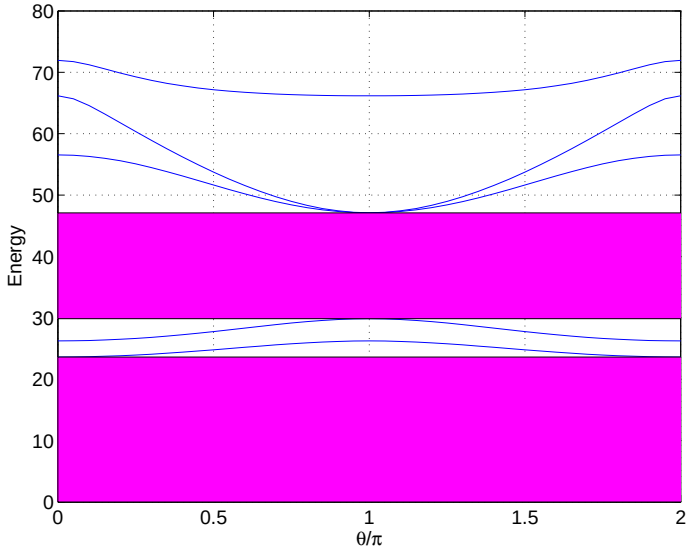

FIG. 2.3. *Dispersion diagram of PA-Two. The first two stop bands are* $(0,23.61_{\pm 0.01})$ *and* $(29.85_{\pm 0.01},47.10_{\pm 0.01})$.

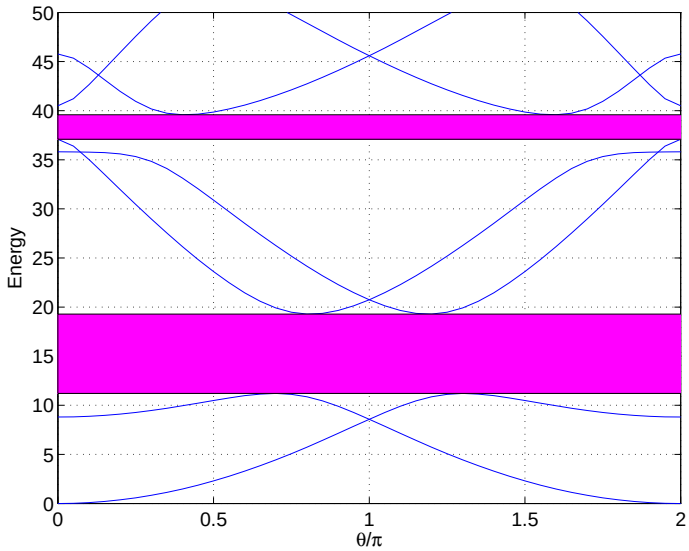

FIG. 2.4. *Dispersion diagram of PA-Three.The first two stop bands are* $(11.20_{\pm 0.01},19.29_{\pm 0.01})$ *and* $(37.08_{\pm 0.01},39.58_{\pm 0.01})$.

3. The limiting absorption principle. The first problem we are facing is how to guarantee the well-posedness of the Helmholtz equation (2.1), which naturally arises due to the absence of a radiation-like condition at infinity. Although the constant coefficient case with separable geometries is well solved, this problem is not trivial at all and largely remains open for the variable coefficient Helmholtz equation.

There are at least three methods of possibly deriving a unique solution of the Helmholtz equation in unbounded domains: asymptotic radiation condition, limiting absorption principle and limiting amplitude principle [49]. In this paper we employ the *limiting absorption principle* (LABP). The LABP is said to hold at $k>0$ if and only if for any $f_0(u)\in L^2(\Gamma_0)$ (take $f_0(u)$ as a unity), the solution $u^\epsilon\in H^1(\Omega)$ of the following *damped Helmholtz equation*

$$\Delta u^\epsilon+(k^2+i\epsilon)n^2u^\epsilon=0 \tag{3.1}$$

with the boundary condition

$$f_0(u^\epsilon)=f_0(u),$$

converges to a unique solution $u\in H^1_{loc}(\Omega)$ of the Helmholtz equation (2.1), and the outgoing Sommerfeld datum $g_0(u^\epsilon)=\mathcal{A}^\epsilon_{inf}f_0(u^\epsilon)$ also converges to the unique function $g_0(u)$. This makes it possible to define a *Sommerfeld-to-Sommerfeld* (StS) mapping $\mathcal{A}_{inf}$ as the limit of $\mathcal{A}^\epsilon_{inf}$, which maps $f_0(u)$ to $g_0(u)$, namely,

$$g_0(u)=\mathcal{A}_{inf}f_0(u).$$

Let us start considering PA-One first. In this case the separation of variables method is available. We set

$$u^\epsilon=\sum_{n=0}^{+\infty}u^{\epsilon,n}\cos(n\pi y)$$

and

$$f_0(u)=\sum_{n=0}^{+\infty}f_0(u^n)\cos(n\pi y),\qquad g_0(u^\epsilon)=\sum_{n=0}^{+\infty}g_0(u^{\epsilon,n})\cos(n\pi y).$$

Then (3.1) is transformed into a sequence of ODE problems:

$$u^{\epsilon,n}_{xx}+(k^2+i\epsilon-n^2\pi^2)u^{\epsilon,n}_{xx}=0,\quad f_0(u^{\epsilon,n})=f_0(u^n),\qquad \forall n=0,1,\ldots.$$

The bounded solutions of the above problems are

$$u^{\epsilon,n}=\frac{f_0(u^n)}{i\sqrt{k^2+i\epsilon-n^2\pi^2}+ik}\,e^{i\sqrt{k^2+i\epsilon-n^2\pi^2}x}.$$

Hence, we have

$$g_0(u^{\epsilon,n})=\frac{i\sqrt{k^2+i\epsilon-n^2\pi^2}-ik}{i\sqrt{k^2+i\epsilon-n^2\pi^2}+ik}\,f_0(u^n),$$

and

$$g_0(u^n)\overset{def}{=}\lim_{\epsilon\to0}g_0(u^{\epsilon,n})=\frac{i\sqrt{k^2-n^2\pi^2}-ik}{i\sqrt{k^2-n^2\pi^2}+ik}\,f_0(u^n). \tag{3.2}$$

Besides, it is straightforward to verify that

$$g_0(u^{\epsilon,n})=g_0(u^n)+\begin{cases}\dfrac{2\sqrt{i\epsilon}f_0(u^n)}{k}+O(\epsilon), & k=n\pi,\\[2ex] \dfrac{ik\epsilon f_0(u^n)}{(\sqrt{k^2-n^2\pi^2}+k)^2\sqrt{k^2-n^2\pi^2}}+O(\epsilon^2), & k\neq n\pi.\end{cases} \tag{3.3}$$

The expression (3.3) states that the convergence rate of $g_0(u^\epsilon)$ to

$$g_0(u) = \sum_{n=0}^{+\infty} g_0(u^n)\cos(n\pi y)$$

is of first order with respect to ϵ if k is unequal to any $n\pi$ with $n \geq 0$. If k is equal to some $n_0\pi$, which implies the resonance of the n_0-th mode in the y-direction, the convergence rate would degenerate to half order. But the LABP holds independent of the wavenumber k.

Based on the above analysis, we conjecture that, under some mild restrictions on the geometry and the refraction index function, the LABP holds for every $k > 0$ for more general semi-infinite periodic arrays. Some numerical evidences will be reported in the end of this section.

The LABP itself suggests a method for deriving the exact StS mapping on the left boundary Γ_0: first compute the exact StS mapping of the problem (3.1) for a given ϵ, denoted by $\mathcal{A}^\epsilon_{inf}$, and then let ϵ tend to zero. In [10] the authors proposed a fast evaluation method for the exact StS mapping of the damped Helmholtz equation (3.1). The basic idea is as follows. For any $N > 0$, the damped Helmholtz equation (3.1) is well-posed on the domain $\cup_{j=0}^{N-1} \mathrm{C}_j$, with the incoming Sommerfeld data f_0^ϵ and g_N^ϵ prescribed at the boundaries Γ_0 and Γ_N. Thus there are four linear scattering operators $\mathcal{A}_N^\epsilon$, $\mathcal{B}_N^\epsilon$, $\mathcal{C}_N^\epsilon$ and $\mathcal{D}_N^\epsilon$ satisfying

$$g_0^\epsilon = \mathcal{A}_N^\epsilon f_0^\epsilon + \mathcal{B}_N^\epsilon g_N^\epsilon, \qquad f_N^\epsilon = \mathcal{C}_N^\epsilon f_0^\epsilon + \mathcal{D}_N^\epsilon g_N^\epsilon.$$

Since g_N^ϵ goes to zero exponentially fast as N tends to infinity, it is reasonable to expect that $\mathcal{A}_N^\epsilon$ converges and the limit is just the exact StS mapping $\mathcal{A}^\epsilon_{inf}$. To make this paper self-contained, we explain in the appendix the *fast doubling procedure* [10] for deriving these scattering operators. This scheme needs only $O(\log_2 N)$ operations.

In Fig. 3.1 we plot the relative errors of the scattering operators $\mathcal{A}_N^\epsilon$ compared to the reference operator $\mathcal{A}^\epsilon_{ref}$, which is obtained by using the doubling technique 20 times, i.e., $N = 2^{20}$. Since FEM is used, the scattering operators are approximated by matrices of rank 65×65. We could see that the doubling technique really leads to an efficient algorithm. Also notice that when k^2 lies in the stop bands, for example $k^2 = 23, 31$, $\mathcal{A}_N$ itself converges as N goes to infinity. This implies that when k^2 is in the stop bands, we could derive the StS mapping directly without considering the LABP.

Next we explain how to let ϵ tend to zero. In light of the expression (3.3), if the resonance does not occur, the exact StS mapping $\mathcal{A}_{inf}$ is expected to bear an asymptotic expansion like

$$\mathcal{A}^\epsilon_{inf} = \mathcal{A}_{inf} + \epsilon \mathcal{A}^{(1)}_{inf} + \epsilon^2 \mathcal{A}^{(2)}_{inf} + \cdots. \tag{3.4}$$

Thus in most cases, the convergence rate of the LABP is of first order. This observation is supported by the numerical evidences shown in Fig. 3.2. Note that the convergence rate could be improved by standard extrapolation techniques. In Fig. 3.3 we show the errors of the StS operators extrapolated once to the reference operator, which is obtained by using extrapolations twice and setting a small damping parameter $\epsilon_0 = 0.00125$. We could see that the accuracy is greatly improved, and second order rate can be clearly observed. We should also notice that if k is close to a resonance wave number, for example $k^2 = 23.61$, 47.1, the asymptotic convergence rate could only manifest for sufficiently small damping parameters.

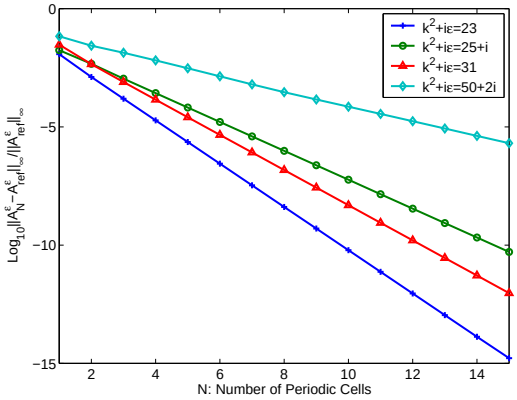

FIG. 3.1. *Relative errors of* $\mathcal{A}^{\epsilon}_{N}$ *to the reference StS mapping* $\mathcal{A}^{\epsilon}_{ref}$*, which is obtained by setting* $N=2^{20}$.

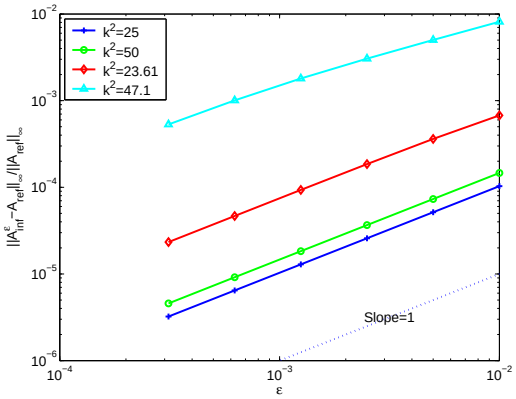

FIG. 3.2. *The reference operator* $\mathcal{A}_{ref}$ *is obtained by setting* $\epsilon=10^{-7}$.

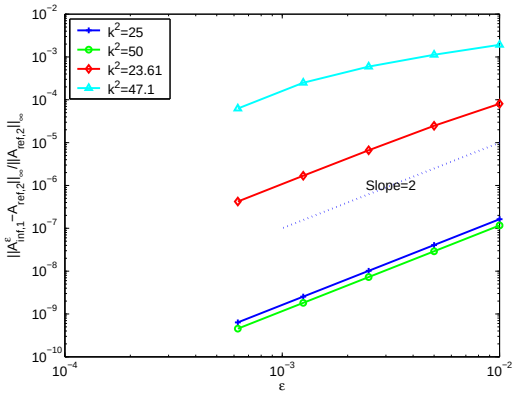

FIG. 3.3. *The reference matrix* $\mathcal{A}_{ref,2}$ *is obtained by using extrapolation technique twice with* $\epsilon_0=0.00125$*, i.e.,* $\mathcal{A}_{ref,2}=\mathcal{A}^{\epsilon_0}_{inf}/3-2\mathcal{A}^{\epsilon_0/2}_{inf}+8\mathcal{A}^{\epsilon_0/4}_{inf}/3$. $\mathcal{A}^{\epsilon}_{inf,1}=-\mathcal{A}^{\epsilon}_{inf}+2\mathcal{A}^{\epsilon/2}_{inf}$ *is obtained by using extrapolation technique once.*

4. Asymptotic behavior of an LABP solution. The last section showed that if k is not a resonance wave number, the extrapolation technique could yield very accurate solution. Obviously this algorithm needs to evaluate the scattering operators for a sequence of ϵ, and this turns out to be computationally quite expensive. Besides, though the chance of k being a resonance wave number is very rare, if k is close to a resonance wave number, the extrapolation method could not present very accurate result. In this section we will develop a new method by directly using the scattering operators for the undamped Helmholtz equation.

Recall from the last section that when k^2 lies in the stop bands, the exact StS mapping could be computed by the doubling technique without using the LABP. This is due to the fact that the solution lies in $L^2(\Omega)$, and thus it decays exponentially fast at infinity. If k^2 lies in the pass bands (complementary energy intervals of stop bands), in general an LABP solution cannot be expected to decay. Our basic idea is to separate those traveling (not-decaying) waves and evanescent (decaying) waves, and handle them by different means.

First let us introduce some notations. Suppose u and v are two solutions of the Helmholtz equation (2.1). Define the *co-related energy flux* of u and v as

$$\mathcal{E}(u,v) = -2ik\left[(u_x,v)_{\Gamma_j} - (u,v_x)_{\Gamma_j}\right] = (f(u),f(v))_{\Gamma_j} - (g(u),g(v))_{\Gamma_j}.$$

Besides, the energy flux of u is defined as $\mathcal{E}(u,u)$, which is also equal to

$$\mathcal{E}(u,u) = 4k\,\mathrm{Im}\int_{\Gamma_j} u_x\bar{u}\,dy.$$

We should remark that the co-related energy flux does not rely on the choice of Γ_j. Moreover, $\mathcal{E}(\cdot,\cdot)$ defines a sesquilinear form.

A nontrivial solution u of the Helmholtz equation (2.1) or (3.1) is regarded as a *Bloch wave* associated with the *Floquet multiplier* $\alpha\in\mathbb{C}$ if it satisfies the following two conditions

$$u|_{\Gamma_{i+1}} = \alpha u|_{\Gamma_i}, \qquad u_x|_{\Gamma_{i+1}} = \alpha u_x|_{\Gamma_i}, \qquad \forall i = 0,1,\ldots.$$

We denote by $\mathbb{F}$ the set of all Floquet factors. A Bloch wave is referred to as evanescent, traveling, or anti-evanescent if the associated Floquet multiplier α satisfies $|\alpha|<1$, $|\alpha|=1$, or $|\alpha|>1$. If $|\alpha|=1$, we refer to α as a *unitary Floquet multiplier*. The set of unitary Floquet multipliers is denoted by $\mathbb{UF}$. Note that the Floquet factor cannot be zero due to the mentioned Holmgren uniqueness theorem. For any $\alpha\in\mathbb{F}$, all associated Bloch waves together with zero function form a linear space. This space, denoted by $\mathbb{E}_\alpha$, is called an (α-*periodic*) *eigenfunction space*. Here we list a couple of propositions about the Floquet theory from [29].

Proposition 4.1. *If $\alpha\in\mathbb{F}$, then $1/\alpha\in\mathbb{F}$ either.*

Proposition 4.2. *$\mathbb{UF}$ is a finite set. For any $\alpha\in\mathbb{UF}$, $N_\alpha = \dim\mathbb{E}_\alpha < +\infty$.*

Proposition 4.3. *Given two Floquet multipliers α_j and α_k, and two functions $\varphi_j\in\mathbb{E}_{\alpha_j}$ and $\varphi_k\in\mathbb{E}_{\alpha_k}$. If $\alpha_j\alpha_k^*\neq 1$, then $\mathcal{E}(\varphi_i,\varphi_j)=0$.*

Proposition 4.4. *If u is an LABP solution, then the energy flux of u is nonnegative.*

Obviously, an LABP solution u cannot include the anti-evanescent Bloch waves, thus asymptotically, u is a combination of traveling Bloch waves. It is known that not every traveling Bloch wave is an LABP solution. We need to pick out those compatible with the LABP. To get some insight, let us consider the homogeneous waveguide problem.

Suppose $k=\pi$. Then the traveling Bloch wave space is given by

$$\mathrm{Span}\{e^{-i\pi x}, e^{i\pi x}, \cos(\pi y)\}.$$

If the x-period L is set as a non-integer positive number, then we get three unitary Floquet multipliers: $e^{-i\pi L}$ associated with $\mathrm{Span}\{e^{-i\pi x}\}$, $e^{i\pi L}$ with $\mathrm{Span}\{e^{i\pi x}\}$ and, 1 with $\mathrm{Span}\{\cos(\pi y)\}$. Since

$$\mathcal{E}(e^{-i\pi x}, e^{-i\pi x}) = 4\pi\,\mathrm{Im}\int_0^1 (-i\pi e^{-i\pi x})e^{i\pi x}\,dy\Big|_{x=0} = -4\pi^2,$$

and an LABP solution has a nonnegative energy flux, $e^{-i\pi x}$ is thus not admissible. Comparatively, we have

$$\mathcal{E}(e^{i\pi x}, e^{i\pi x}) = 4\pi\,\mathrm{Im}\int_0^1 (i\pi e^{i\pi x})e^{-i\pi x}\,dy\Big|_{x=0} = 4\pi^2,$$

and

$$\mathcal{E}(\cos(\pi y), \cos(\pi y)) = 4\pi\,\mathrm{Im}\int_0^1 (0)e^{i\pi x}\,dy\Big|_{x=0} = 0.$$

The problem appears when L is taken as an integer. For example, let us take $L=1$. In this case there are two unitary Floquet multipliers 1 and -1, namely,

$$\begin{aligned}\alpha_1 &= -1 \longleftrightarrow \mathbb{E}_{\alpha_1} = \mathrm{Span}\{e^{-i\pi x},\ e^{i\pi x}\},\\ \alpha_2 &= \ \ 1 \longleftrightarrow \mathbb{E}_{\alpha_2} = \mathrm{Span}\{\cos(\pi y)\}.\end{aligned}$$

$\mathbb{E}_{\alpha_2}$ represents a resonance space, and two-dimensional space $\mathbb{E}_{\alpha_1}$ contains both the left-going and right-going traveling waves. The problem is how to classify these two kind of waves. One may say the energy principle could still work, since obviously the Bloch wave $e^{i\pi x}$ is outgoing, and $e^{-i\pi x}$ is incoming. But the question is that $\mathbb{E}_{\alpha_1}$ may have different basis representation, for example,

$$\mathbb{E}_{\alpha_1} = \mathrm{Span}\{e^{-i\pi x}+2e^{i\pi x},\ e^{-i\pi x}+3e^{i\pi x}\} = \mathrm{Span}\{e^{i\pi x}+2e^{-i\pi x},\ e^{i\pi x}+3e^{-i\pi x}\}.$$

For the first representation, both basis functions are right-going, and for the second, both are left-going. However, generally we could not distinguish an LABP outgoing traveling wave only through its energy flux.

The above problem becomes even more severe if we take $L=2$. In this case there exists only one unitary Floquet multiplier

$$\alpha = 1 \longleftrightarrow \mathbb{E}_{\alpha} = \mathrm{Span}\{e^{-i\pi x},\ e^{i\pi x}, \cos(\pi y)\}.$$

It is not hard to find different basis representations for $\mathbb{E}_{\alpha}$, which have completely different signs of energy flux. As a conclusion, if α is a unitary Floquet multiplier and the associated eigenfunction space $\mathbb{E}_{\alpha}$ is multi-dimensional, we have to resort to other criterion to determine the LABP right-going Bloch waves.

Let us remark here that for a three-dimensional waveguide problem, the chance for $\mathbb{E}_{\alpha}$ being multi-dimensional is absolutely not rare, though it seems true for two-dimensional waveguide problems.

Suppose $\alpha\in\mathbb{UF}$, and $\{\varphi_j\}_{j=1}^{N_\alpha}$ constitute a set of basis functions of $\mathbb{E}_\alpha$, *orthonormal* w.r.t. the n^2-weighted inner product $(\cdot,\cdot)_{n^2}$ defined as

$$(\varphi_j,\varphi_k)_{n^2}=\int_{C_0} n^2\varphi_j\bar{\varphi}_k\,dy.$$

We define the *energy flux matrix* $M=(m_{jk})$ as

$$m_{jk}=\mathcal{E}(\varphi_j,\varphi_k),\qquad \forall j,k=1,2,\cdots,N_\alpha.$$

It is easy to verify that M is a Hermitian matrix, which implies the existence of a unitary matrix U, such that

$$U^\top M\bar{U}=\Lambda=\mathrm{diag}(\lambda_1,\lambda_2,\ldots,\lambda_{N_\alpha}),$$

where λ_j are real eigenvalues of M ordered by

$$\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_{m_1}>0=\lambda_{m_1+1}=\cdots=\lambda_{m_2}=0>\lambda_{m_2+1}\geq\cdots\geq\lambda_{N_\alpha}.$$

We introduce a new set of basis function $\{\psi_j\}_{j=1}^{N_\alpha}$ as

$$(\psi_1,\ldots,\psi_{N_\alpha})=(\varphi_1,\ldots,\varphi_{N_\alpha})U,$$

which will be referred to as a *canonical set of basis functions* of $\mathbb{E}_\alpha$. Now we could separate $\mathbb{E}_\alpha$ into three parts, i.e.,

$$\mathbb{E}_\alpha=\mathbb{R}_\alpha\oplus\mathbb{S}_\alpha\oplus\mathbb{L}_\alpha,$$

with

$$\mathbb{R}_\alpha=\mathrm{Span}\{\psi_1,\cdots,\psi_{m_1}\},\qquad \mathbb{S}_\alpha=\mathrm{Span}\{\psi_{m_1+1},\cdots,\psi_{m_2}\},$$

$$\mathbb{L}_\alpha=\mathrm{Span}\{\psi_{m_2+1},\cdots,\psi_{N_\alpha}\}.$$

Proposition 4.5. *For any $\alpha\in\mathbb{E}_\alpha$, $\{\lambda_j\}_{j=1}^{N_\alpha}$ are invariant quantities, and $\mathbb{R}$, $\mathbb{S}$ and $\mathbb{L}$ are invariant subspaces of $\mathbb{E}_\alpha$. Besides, for any $\varphi_1\in\mathbb{R}_\alpha$, $\varphi_2\in\mathbb{S}_\alpha$, $\varphi_3\in\mathbb{L}_\alpha$, we have*

$$\mathcal{E}(\varphi_1,\varphi_1)>0,\qquad \mathcal{E}(\varphi_2,\varphi_2)=0,\qquad \mathcal{E}(\varphi_3,\varphi_3)<0.$$

For the homogeneous waveguide problem, it is straightforward to verify that $\mathbb{R}_\alpha$ is the admissible LABP Bloch wave space with positive energy flux. $\mathbb{S}_\alpha$ is the resonance wave space, which is also admissible to the LABP. Note that if $\mathbb{S}_\alpha$ is excluded from the asymptotic solution space, the Helmholtz equation would loose solvability for some incoming Sommerfeld data f_0.

Based on these facts, for a general semi-infinite periodic array, we make the following conjecture.

Conjecture 4.6. *Suppose $\alpha_1,\ldots,\alpha_M$ are all unitary Floquet multipliers, and $\varphi_1^{\alpha_j},\ldots,\varphi_{N_{\alpha_j}}^{\alpha_j}$ constitute a set of orthonormal basis functions of $\mathbb{R}_{\alpha_j}\oplus\mathbb{S}_{\alpha_j}$. Then asymptotically, any LABP solution u lies in the space*

$$\mathrm{Span}\{\varphi_k^{\alpha_j}|j=1,\ldots,M,k=1,\ldots,N_{\alpha_j}\}. \tag{4.1}$$

Although we have no proof of this conjecture yet, its validity is strongly supported by the numerical tests given in the next section. Let us remark here that according to Proposition 4.3, $\{\varphi_k^{\alpha_j}\}_{j=1,k=1}^{M,N_{\alpha_j}}$ in fact constitute a set of basis functions of the LABP right-going Bloch wave space.

5. Evaluation of the exact StS mapping. Based on Conjecture 4.6, we know when N is large, asymptotically,

$$f_N(u)\approx\sum_{j=1}^{M}\sum_{k=1}^{N_{\alpha_j}}t_k^j f_0(\varphi_k^{\alpha_j}),\qquad g_N(u)\approx\sum_{j=1}^{M}\sum_{k=1}^{N_{\alpha_j}}t_k^j g_0(\varphi_k^{\alpha_j}).$$

Or in an abbreviated vector form,

$$f_N(u)\approx FT,\qquad g_N(u)\approx GT, \tag{5.1}$$

where

$$F=(F_1,\cdots,F_M),\quad G=(G_1,\cdots,G_M),\quad T=(T_1,\cdots,T_M)^\top$$

with

$$F_j=(f_0(\varphi_1^{\alpha_j}),\cdots,f_0(\varphi_{N_{\alpha_j}}^{\alpha_j})),\ G_j=(g_0(\varphi_1^{\alpha_j}),\cdots,g_0(\varphi_{N_{\alpha_j}}^{\alpha_j})),\ T_j=(t_1^{\alpha_j},\cdots,t_{N_{\alpha_j}}^{\alpha_j}), \tag{5.2}$$

Recall that

$$g_0(u)=\mathcal{A}_N f_0(u)+\mathcal{B}_N g_N(u),\qquad f_N(u)=\mathcal{C}_N f_0(u)+\mathcal{D}_N g_N(u).$$

Using (5.1) T could be derived by the least square method as

$$T\approx(F-\mathcal{D}_N G)^{-1}\mathcal{C}_N f_0(u). \tag{5.3}$$

Here, $^{-1}$ denotes the pseudo-inverse operator. We then have

$$g_0(u)=\mathcal{A}_N f_0(u)+\mathcal{B}_N g_N(u)\approx(\mathcal{A}_N+\mathcal{B}_N G(F-\mathcal{D}_N G)^{-1}\mathcal{C}_N)f_0(u),$$

which means that by putting

$$\tilde{\mathcal{A}}_N=\mathcal{A}_N+\mathcal{B}_N G(F-\mathcal{D}_N G)^{-1}\mathcal{C}_N,$$

the limit of $\tilde{\mathcal{A}}_N$ would give the exact StS mapping $\mathcal{A}_{inf}$ on the left boundary Γ_0.

The key step to implement the above algorithm is to derive a canonical set of basis functions for all unitary Floquet multipliers. Or more explicitly, we need to compute the functions F_j and G_j defined in (5.2). This objective can be achieved by several steps:

1. Solve the generalized eigenvalue problem

$$\begin{pmatrix}-\mathcal{A}_1 & I\\ -\mathcal{C}_1 & 0\end{pmatrix}\begin{pmatrix}f_0\\ g_0\end{pmatrix}=\alpha\begin{pmatrix}0 & \mathcal{B}_1\\ -I & \mathcal{D}_1\end{pmatrix}\begin{pmatrix}f_0\\ g_0\end{pmatrix}$$

   to obtain all (different) unitary Floquet multipliers $\{\alpha_j\}_{j=1}^M$ and their associated generalized eigenfunctions $(f_{0,k}^{\alpha_j},g_{0,k}^{\alpha_j})$, $k=1,\cdots,N_{\alpha_j}$.
2. If $\mathbb{E}_{\alpha_j}$ is one-dimensional, i.e., $N_{\alpha_j}=1$, compute the energy flux of the eigenfunction φ_1^j associated with the Sommerfeld data $(f_{0,1}^{\alpha_j},g_{0,1}^{\alpha_j})$ by

$$\mathcal{E}(\varphi_1^j,\varphi_1^j)=(f_{0,1}^{\alpha_j},f_{0,1}^{\alpha_j})_{\Gamma_0}-(g_{0,1}^{\alpha_j},g_{0,1}^{\alpha_j})_{\Gamma_0}.$$

   If and only if $\mathcal{E}(\varphi_1^j,\varphi_1^j)\geq 0$, then φ_1^j is an admissible LABP traveling Bloch wave, i.e., $F_j=(f_{0,1}^{\alpha_j})$, $G_j=(g_{0,1}^{\alpha_j})$. Otherwise, $F_j=G_j=\emptyset$.

3. If $\mathbb{E}_{\alpha_j}$ is multi-dimensional, i.e., $N_{\alpha_j}>1$, derive a set of orthonormal eigenfunctions $\{\varphi_k^{\alpha_j}\}_{k=1}^{N_{\alpha_j}}$ of the following problem

$$\begin{aligned}&\Delta u+k^2n^2u=0,\\&u|_{\Gamma_1}=\alpha_j u|_{\Gamma_0},\quad u_x|_{\Gamma_1}=\alpha_j u_x|_{\Gamma_0}.\end{aligned}$$

Compute the associated Sommerfeld data $\{f_0(\varphi_k^{\alpha_j})\}$ and $\{g_0(\varphi_k^{\alpha_j})\}$. Compute the energy matrix $M=(m_{kl})$ with

$$m_{kl}=(f_0(\varphi_k^{\alpha_j}),f_0(\varphi_l^{\alpha_j}))_{\Gamma_0}-(g_0(\varphi_k^{\alpha_j}),g_0(\varphi_l^{\alpha_j}))_{\Gamma_0},\quad \forall k,l=1,\cdots,N_{\alpha_j}.$$

Find a unitary matrix $U=(u_{lk})$ to diagonalize M, such that

$$U^\top M\bar{U}=\Lambda=\mathrm{diag}(\lambda_1,\lambda_2,\ldots,\lambda_{N_{\alpha_j}}),$$

where λ_j are real eigenvalues of M ordered by

$$\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_{m_1}>0=\lambda_{m_1+1}=\cdots=\lambda_{m_2}=0>\lambda_{m_2+1}\geq\cdots\geq\lambda_{N_{\alpha_j}}.$$

Set $F_j=(F_j^1,\cdots,F_j^{m_2})$ and $G_j=(G_j^1,\cdots,G_j^{m_2})$ with

$$F_j^k=\sum_{l=1}^{N_{\alpha_j}}f_0(\varphi_l^{\alpha_j})u_{lk},\quad G_j^k=\sum_{l=1}^{N_{\alpha_j}}g_0(\varphi_l^{\alpha_j})u_{lk},\quad \forall k=1,\cdots,m_2.$$

4. Finally, set $F=(F_1,\cdots,F_N)$ and $G=(G_1,\cdots,G_N)$.

In the following we will report our numerical tests. For simplicity, we refer to the StS mapping derived with the LABP as LABP-StS, and the StS mapping based on the asymptotic expansion of the traveling Bloch waves as ASYM-StS. First we consider the PA-One. In this case the analytical StS mapping is available. For the n-th mode in the y-direction, the exact StS mapping is given as in (3.2). The computed StS mapping, no matter which method is employed, is diagonalizable. In Table 5.1 we list the errors of ASYM-StS. We see generally the asymptotic method presents very accurate results except on the resonance wave number. For example, if $k=\pi$, the first y-mode is resonant.

	$n=0$	$n=1$	$n=2$	$n=3$	$n=4$
$k=\pi$	1.50(-9)	7.58(-6)	2.13(-12)	5.44(-13)	2.28(-13)
$k=\frac{5\pi}{4}$	4.60(-9)	1.78(-9)	3.52(-12)	8.74(-13)	3.24(-13)
$k=\sqrt{2}\pi$	7.02(-12)	1.07(-9)	1.31(-11)	2.80(-12)	1.00(-12)
$k=\sqrt{3}\pi$	5.91(-13)	9.44(-13)	3.23(-12)	5.40(-13)	2.10(-13)

TABLE 5.1. *Errors of Direct computation.*

In Table 5.2 we list the errors of the LABP-StS. They are derived with two times of extrapolation. We see that except at the resonance wave numbers, this method presents the results at least of the same quality of those derived by the asymptotic method. But when resonance occurs, the extrapolation technique is only of little use. In order to obtain high accuracy, one has to make the damping parameter very small, but this probably implies a numerical stability problem.

For the other two periodic structures PA-Two and PA-Three, no analytical expression is available on the exact StS mapping. We compare the numerical solutions by two different methods. From Table 5.3-5.4, we could conclude in principle these two methods bring the same results. When k is away from the resonance wave number, these two methods present the results of same quality. But their difference becomes big when k approaches the resonance wave number. Considering the results for the homogeneous waveguide problem, we thus believe at the resonance wave numbers, the asymptotic method presents better solution.

	$n=0$	$n=1$	$n=2$	$n=3$	$n=4$
$k=\pi$	5.03(-9)	5.68(-3)	2.26(-12)	7.51(-13)	2.39(-13)
$k=\frac{5\pi}{4}$	3.53(-12)	7.30(-12)	3.43(-12)	8.22(-13)	2.74(-13)
$k=\sqrt{2}\pi$	6.91(-12)	1.52(-8)	1.26(-11)	2.99(-12)	1.06(-12)
$k=\sqrt{3}\pi$	1.07(-12)	1.49(-12)	3.40(-12)	5.82(-13)	2.37(-13)

TABLE 5.2. $\epsilon=0.00125$. *Extrapolation.*

	$k^2=25$	$k^2=50$	$k^2=23.61$	$k^2=47.1$
Relative error	1.31(-12)	3.26(-12)	3.89(-8)	6.76(-5)

TABLE 5.3. $\epsilon=0.00125$. *Comparison. PA-Two*

	$k^2=5$	$k^2=25$	$k^2=11.20$	$k^2=19.29$
Relative error	9.58(-13)	9.26(-13)	7.16(-9)	6.23(-10)

TABLE 5.4. $\epsilon=0.00125$. *Comparison. PA-Three.*

Conclusion. We have considered the Helmholtz equation in the semi-infinite periodic array in this paper. Since no radiation-like boundary condition is specified at infinity, the Helmholtz equation is in general not well-posed. To solve this problem we employed the limiting absorption principle. We have proposed a new algorithm which combines the doubling procedure and the extrapolation technique to obtain high-accuracy approximation to the exact StS mappings. Considering the computational complexity, we present another method which uses the asymptotic behavior of a limiting absorption principle solution. Though we could not prove, the validity of this method is strongly supported by our numerical evidences.

We believe these two methods could be extended to more complicated wave-like equations, such as Maxwell's equations and elastic wave equations. Besides, we have left the relevant theoretical problems open in this paper. Hopefully we could make some progress on these issues in the near future.

Appendix—The doubling procedure. On the vertical boundary segments Γ_i we define two *Robin data* as

$$f_i=(\partial_x+ik)u|_{\Gamma_i},\qquad g_i=(\partial_x-ik)u|_{\Gamma_i}. \tag{5.4}$$

For any given boundary data f_i and g_{i+k}, $i\geq 0$, $k\geq 1$, the Helmholtz equation (2.1) is uniquely solvable on $\cup_{l=i}^{i+k-1}C_l$, cf. [10, Lemma A]. Due to the assumption on the boundary conditions, there exists four linear operators $\mathcal{A}_k$, $\mathcal{B}_k$, $\mathcal{C}_k$ and $\mathcal{D}_k$ satisfying

$$g_i=\mathcal{A}_k f_i+\mathcal{B}_k g_{i+k},\qquad f_{i+k}=\mathcal{C}_k f_i+\mathcal{D}_k g_{i+k}. \tag{5.5}$$

From the numerical point of view, these operators can be derived by an appropriate spatial discretization in the domain $\cup_{k=0}^{j-1}C_k$. But if k is large, a vast number of unknowns would get involved, which leads to a high computational effort. As revealed in [10], these operators can be obtained very efficiently with a *smart doubling procedure*.

The essential idea of this doubling procedure is based on the following recursive relations. Suppose for $k\in\{m,n\}$, the operators $\mathcal{A}_k$, $\mathcal{B}_k$, $\mathcal{C}_k$ and $\mathcal{D}_k$ have already been obtained. By (5.5) we have

$$\begin{aligned} g_i&=\mathcal{A}_m(\mathcal{C}_n f_{i-n}+\mathcal{D}_n g_i)+\mathcal{B}_m g_{i+m},\\ f_i&=\mathcal{C}_n f_{i-n}+\mathcal{D}_n(\mathcal{A}_m f_i+\mathcal{B}_m g_{i+m}).\end{aligned}$$

It is easy to prove that $I-\mathcal{A}_m\mathcal{D}_n$ and $I-\mathcal{D}_n\mathcal{A}_m$ (I denotes the identity operator) are invertible, cf. [10, Lemma B]. Thus then,

$$g_i=\mathcal{A}^*_{n,m}f_{i-n}+\mathcal{B}^*_{n,m}g_{i+m},\quad f_i=\mathcal{C}^*_{n,m}f_{i-n}+\mathcal{D}^*_{n,m}g_{i+m}, \tag{5.6}$$

where

$$\begin{aligned} \mathcal{A}^*_{n,m}&=(I-\mathcal{A}_m\mathcal{D}_n)^{-1}\mathcal{A}_m\mathcal{C}_n,\quad \mathcal{B}^*_{n,m}=(I-\mathcal{A}_m\mathcal{D}_n)^{-1}\mathcal{B}_m,\\ \mathcal{C}^*_{n,m}&=(I-\mathcal{D}_n\mathcal{A}_m)^{-1}\mathcal{C}_n,\quad \mathcal{D}^*_{n,m}=(I-\mathcal{D}_n\mathcal{A}_m)^{-1}\mathcal{D}_n\mathcal{B}_m.\end{aligned}$$

Substituting expressions (5.6) into (5.5) gives

$$\begin{aligned} g_{i-n}&=\mathcal{A}_n f_{i-n}+\mathcal{B}_n(\mathcal{A}^*_{n,m}f_{i-n}+\mathcal{B}^*_{n,m}g_{i+m}),\\ f_{i+m}&=\mathcal{C}_m(\mathcal{C}^*_{n,m}f_{i-n}+\mathcal{D}^*_{n,m}g_{i+m})+\mathcal{D}_m g_{i+m},\end{aligned}$$

which imply

$$\begin{aligned} \mathcal{A}_{m+n}&=\mathcal{A}_n+\mathcal{B}_n\mathcal{A}^*_{n,m},\quad \mathcal{B}_{m+n}=\mathcal{B}_n\mathcal{B}^*_{n,m},\\ \mathcal{C}_{m+n}&=\mathcal{C}_m\mathcal{C}^*_{n,m},\quad \mathcal{D}_{m+n}=\mathcal{D}_m+\mathcal{C}_m\mathcal{D}^*_{n,m}.\end{aligned} \tag{5.7}$$

Hence, for any fixed cell number N, the operators $\mathcal{A}_N$, $\mathcal{B}_N$, $\mathcal{C}_N$, and $\mathcal{D}_N$ can be obtained by the following steps:

1. Derive $\mathcal{A}_1$, $\mathcal{B}_1$, $\mathcal{C}_1$, and $\mathcal{D}_1$ by the *cell analysis*. If $N=1$, it is done;
2. Write N into *binary form* $(j_L\cdots j_0)_2$, with $L=[\log_2 N]$ and $j_L=1$;
3. Use the relations (5.7) L times by setting $m=n=2^{k-1}$ to get $\mathcal{A}_{2^k}$, $\mathcal{B}_{2^k}$, $\mathcal{C}_{2^k}$, and $\mathcal{D}_{2^k}$ for $k=1,\ldots,L$;
4. For $l=L-1,\ldots,0$, if $j_l\neq 0$, then use (5.7) by setting $m=(j_L\cdots j_{l+1}0\cdots 0)_2$ and $n=2^l$ to obtain $\mathcal{A}_{(j_L\cdots j_l0\cdots0)_2}$, $\mathcal{B}_{(j_L\cdots j_l0\cdots0)_2}$, $\mathcal{C}_{(j_L\cdots j_l0\cdots0)_2}$ and $\mathcal{D}_{(j_L\cdots j_l0\cdots0)_2}$.

The above procedure uses (5.7) at most $2[\log_2 N]$ times, and only $J=[\log_2 N]$ times if $N=2^J$.

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