Scattering Problems in Periodic Media with Local Perturbations

Therese Pollok, Lin Zschiedrich, and Frank Schmidt

Abstract Within this paper we consider scattering problems with periodic exterior domains, modeled by the Helmholtz equation. Most current works on this subject make specific assumptions on the geometry of the periodic cell, e.g. special symmetries or shapes, and cannot be generalized to higher space dimensions in an easy way. In contrast our goal is the realization of an easy dimension independent concept which is valid for all kinds of periodic structures with local defects. We will first give a general analytical formulation and then present an algorithmic realization. At the end of the paper we will also depict a 1D and 2D example.

1 Introduction and Problem Setting

Periodic structures such as photonic crystals or metamaterials have many applications in modern optic devices due to their optical properties, as for example the occurrence of band gaps, i.e. forbidden frequency ranges, or negative refractive indices. Particularly defects within the periodicity of band gap materials are of special interest since they can be used to manipulate the flow of light efficiently. By disturbing a whole line of unit cells for example one can produce a waveguide for frequencies within the band gap whereas local perturbations yield optical cavities. For more details see for example [1, 4]. We will confine our considerations to local defects, i.e., the perturbation is restricted to a bounded region Ω as illustrated in Fig. 1. Without loss of generality we will further assume, that Ω is contained in one single unit cell C_0.

In real applications photonic crystals often consist of a very large number of unit cells. We will therefore assume that the crystal is of infinite size.

T. Pollok (✉) · L. Zschiedrich · F. Schmidt
Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany
e-mail: pollok@zib.de; zschiedrich@zib.de; frank.schmidt@zib.de

B. Michielsen and J.-R. Poirier (eds.), *Scientific Computing in Electrical Engineering SCEE 2010*, Mathematics in Industry 16, DOI 10.1007/978-3-642-22453-9_8,

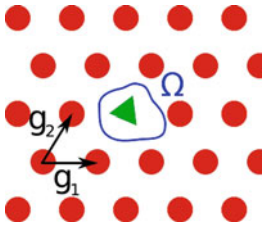

Fig. 1 2D periodic structure with a local perturbation

Furthermore we assume a non-conducting and charge-free medium and a time-harmonic incoming wave and model the scattering problem by the scalar Helmholtz equation $\Delta u(\mathbf{r}) + k^2(\mathbf{r})u(\mathbf{r}) = f(\mathbf{r})$. The material properties thereby are contained in $k^2(\mathbf{r}) = \varepsilon(\mathbf{r})\mu(\mathbf{r})\omega^2$, where ω is the frequency of the incoming wave. The right hand term $f(\mathbf{r})$ is the source term, resulting from the incoming wave (see (5)).

One of the most important works on this subject is the work of P. Joly [3] in which for 2D structures a coupled operator equation system for four operators is derived. It can be decoupled in the special case of so called *double symmetric* refractive indices but is much more involved for the general unsymmetric case. In [2], which is a second important work in this field, only 2D structures are considered which consist of cylinders of refractive index n_i in an elsewise homogeneous medium of refractive index n_e. In view of the development of an universal tool we are interested in an easier and general concept which is independent of the spacial dimension.

2 Scattering Problems

Let u_{in} be an incident wave which satisfies the Helmholtz equation in the exterior domain $\Omega_{\text{ext}} = \mathbb{R}^d \setminus \Omega$:

$$\Delta u_{\text{in}}(\mathbf{r}) + k_{\text{per}}^2(\mathbf{r})u_{\text{in}}(\mathbf{r}) = 0, \tag{1}$$

where k_{per} is an (undisturbed) periodic function with lattice vectors $\mathbf{g}_j$ for $j = 1, \ldots, d$, i.e.,

$$k_{\text{per}}(\mathbf{r} + \mathbf{g}_j) = k_{\text{per}}(\mathbf{r}) \quad \forall \mathbf{r} \in \mathbb{R}^d. \tag{2}$$

Find the scattered wave u_{sc} such that for the total field $u_{\text{tot}} = u_{\text{in}} + u_{\text{sc}}$,

$$\Delta u_{\text{tot}}(\mathbf{r}) + k^2(\mathbf{r})u_{\text{tot}}(\mathbf{r}) = 0 \quad \text{in } \mathbb{R}^d, \tag{3}$$

where

$$k^2(\mathbf{r}) = k_{\text{per}}^2(\mathbf{r}) + k_{\Delta}^2(\mathbf{r}) \tag{4}$$

for a function k_{Δ} with support in Ω. Without loss of generality we assume that Ω is contained in a unit cell of the periodic structure.

By inserting (1) and (4) into (3) one obtains

$$\Delta u_{\text{sc}} + k^2 u_{\text{sc}} = -k_\Delta^2 u_{\text{in}} =: f \quad \text{in } \mathbb{R}^d, \tag{5}$$

with supp $f \subseteq \Omega$.

In order to obtain the physically correct solution we require in addition a radiation condition that ensures that u_{sc} is purely outgoing. For the mathematical formulation of this radiation condition we will use the limiting absorption principle which is part of the next section.

For the sake of simplicity we will omit the subscript of the scattered field u_{sc} and denote it in the following as u.

3 Bloch-Floquet Transform and Limiting Absorption Principle

Due to backscattering off the periodic configuration of materials, distinguishing between incoming and outgoing waves is much more involved than in the homogeneous case. The standard approach to overcome this difficulty is to introduce artificial damping by replacing $k \to k(1 + \mathrm{i}\sigma)$, where $\sigma \in \mathbb{R}_+$ is the damping parameter. The outgoing waves of the damped problem are exponentially decaying for $|\mathbf{r}| \to \infty$ and thus can be distinguished from the exponentially growing incoming waves. This is known as *limiting absorption principle* and was first introduced by Joly [5] and reads:

Find $u \in L^2(\mathbb{R}^d)$ such that

$$\Delta u + k^2(1 + \mathrm{i}\sigma)^2 u = f. \tag{6}$$

Next, we introduce the so-called Bloch-Floquet transform, a second standard technique for the treatment of periodic problems. Its application to the Helmholtz equation leads to boundary value problems with finite computational domains, as detailed in the following.

Let $\mathbf{G} := (\mathbf{g}_1, \ldots, \mathbf{g}_d)$ the matrix consisting of the lattice vectors $\mathbf{g}_j$ (see (2) and Fig. 1) and

$$\Gamma := \left\{ \mathbf{G}\mathbf{n} | \mathbf{n} \in \mathbb{Z}^d \right\}.$$

For exponentially decaying u one can define the Bloch-Floquet transform $\mathrm{Fl}(u) =: \hat{u}$ by

$$\hat{u}(\mathbf{k}_B, \mathbf{r}) := \sum_{\mathbf{d} \in \Gamma} u(\mathbf{r} + \mathbf{d}) \exp(-\mathrm{i}\mathbf{k}_B \cdot \mathbf{d}), \tag{7}$$

where $\mathbf{k}_B \in \mathbb{R}^d$ is called *Bloch vector*. (See [6].)

It can easily be shown that $\hat{u}$ is periodic with respect to $\mathbf{k}_B$: Let $\tilde{\mathbf{g}}_1, \ldots, \tilde{\mathbf{g}}_d$ the *reciprocal lattice vectors*, i.e.

$$\mathbf{g}_i \cdot \tilde{\mathbf{g}}_j = 2\pi \delta_{ij}.$$

Then

$$\hat{u}(\mathbf{k}_B + \tilde{\mathbf{g}}_j, \mathbf{r}) = \hat{u}(\mathbf{k}_B, \mathbf{r}).$$

Hence it is sufficient to consider $\mathbf{k}_B \in \mathrm{BZ}$, where BZ is the so called *first Brillouin zone* which is defined as the primitive unit cell of the reciprocal lattice. The inverse of the Bloch-Floquet transform reads

$$u(\mathbf{r}) = \frac{1}{|BZ|} \int_{\mathrm{BZ}} \hat{u}(\mathbf{k}_B, \mathbf{r}) \mathrm{d}\mathbf{k}_B. \tag{8}$$

Let us now apply the Bloch-Floquet transform to the damped Helmholtz equation (6). It can be easily shown that for the periodic part k_{per} of k,

$$\mathrm{Fl}(k_{\mathrm{per}}^2 u) = k_{\mathrm{per}}^2 \mathrm{Fl}(u). \tag{9}$$

Thus, by using (4) and (9), we obtain

$$\Delta\hat{u} + k_{\mathrm{per}}^2(1 + \mathrm{i}\sigma)^2\hat{u} + \mathrm{Fl}\left(k_\Delta^2(1 + \mathrm{i}\sigma)^2 u\right) = \mathrm{Fl}(f). \tag{10}$$

Without loss of generality we can assume $\Omega \subset C_0$, where C_0 is a unit cell of the periodic structure (otherwise define C_0 as a sufficient large cell). Then for every function g with support in Ω holds $\mathrm{Fl}(g)(\mathbf{k}_B, \mathbf{r}) = g(\mathbf{r})$ for all $\mathbf{r} \in C_0$. Thus we may write

$$\Delta\hat{u} + k_{\mathrm{per}}^2(1 + \mathrm{i}\sigma)^2\hat{u} + k_\Delta^2(1 + \mathrm{i}\sigma)^2 u = f \quad \text{in } \mathrm{BZ} \times C_0. \tag{11}$$

We can obtain an equation for $\hat{u}$ from (10) by applying the inverse transform (8):

$$\Delta\hat{u} + k_{\mathrm{per}}^2(1 + \mathrm{i}\sigma)^2\hat{u} + k_\Delta^2(1 + \mathrm{i}\sigma)^2 \frac{1}{|\mathrm{BZ}|} \int_{\mathrm{BZ}} \hat{u} \mathrm{d}\mathbf{k}_B = f \quad \text{in } \mathrm{BZ} \times C_0. \tag{12}$$

By adding a lattice vector $\mathbf{g}_j$ of the periodic structure to the space argument $\mathbf{r}$ in the definition (7) of the Bloch-Floquet transform we see that $\hat{u}(\mathbf{k}_B, \mathbf{r})$ is *quasi-periodic*:

$$\hat{u}(\mathbf{k}_B, \mathbf{r} + \mathbf{g}_j) = \hat{u}(\mathbf{k}_B, \mathbf{r}) \exp(\mathrm{i}\mathbf{k}_B \cdot \mathbf{g}_j). \tag{13}$$

Equation (13) yields the boundary conditions that enable us to restrict the spacial computational domain to the unit cell C_0. It also tells us how to extend the solution to $\mathbb{R}^d$.

Remark 1. Since any bounded solution $\hat{u}$ of (12) is extended by (13) it remains bounded on $\mathbb{R}^d$. Therefore the solution u of (6) which can be obtained by inverting $\hat{u}$ with (8) is also bounded and thus contains no exponentially growing part. This means that the obtained solution must be outward radiating as demanded.

4 Algorithmic Solution

Equation (12) is a $2d$-dimensional problem since $\hat{u}$ depends on $\mathbf{k}_B$ and $\mathbf{r}$. In the case of $k_\Delta = 0$ (12) would decouple into one d-dimensional boundary value problem

$$\Delta\hat{u}(\mathbf{k}_B, \bullet) + k_{\text{per}}^2(1 + \mathrm{i}\sigma)^2\hat{u}(\mathbf{k}_B, \bullet) = f \qquad \text{in } C_0 \tag{14}$$

$$\hat{u}(\mathbf{k}_B, \mathbf{r} + \mathbf{g}_j) = \hat{u}(\mathbf{k}_B, \mathbf{r}) \exp(\mathrm{i}\mathbf{k}_B \cdot \mathbf{g}_j)$$

for each $\mathbf{k}_B \in \mathrm{BZ}$, which we can solve with standard methods.

Let us now assume we already knew the solution u of the original problem with $k_\Delta \neq 0$. Then we would get from (10)

$$\Delta\hat{u}(\mathbf{k}_B, \bullet) + k_{\text{per}}^2(1 + \mathrm{i}\sigma)^2\hat{u}(\mathbf{k}_B, \bullet) = \tilde{f} \qquad \text{in } C_0 \tag{15}$$

with the new right hand side $\tilde{f} = f - k_\Delta^2(1 + \mathrm{i}\sigma)^2 u$ and we would have again a problem of the same type as (14). This motivates the following iteration:

$u_n = u_0$;
for $n = 0 : \text{max\_iteration\_steps}$ **do**
  $\hat{u} \leftarrow$ solve (15) with $\tilde{f} = f - k_\Delta^2(1 + \mathrm{i}\sigma)^2 u_n$;
  $u_{n+1} \leftarrow \text{FloquetInvert}(\hat{u})$;
end for

As initial value for the iteration we choose $u_0 = 0$. This implies that in the first iteration step the algorithm solves the unperturbed periodic problem.

To solve (15) for one specific value of $\mathbf{k}_B$ we use a standard finite element method with quasi-periodic ansatz functions

$$\phi(\mathbf{r} + \mathbf{g}_j) = \phi(\mathbf{r}) \exp(\mathrm{i}\mathbf{k}_B \cdot \mathbf{g}_j) \text{ for } j = 1, \ldots, d. \tag{16}$$

This special choice of ansatz functions eliminates the boundary integral from the variational formulation of (15). The numerical integration in (8) requires the evaluation of (15) for several values $\mathbf{k}_B$ which means computing several finite element solutions per iteration step. To keep the computational effort low we used an adaptive integration formula that uses an unstructured grid. The choice of the damping parameter σ influences the effort required for the numerical integration, since $\sigma = 0$ would yield a solution with singularities which are smoothed when increasing σ. Therefore the choice of σ is a tradeoff between low integration costs and perturbation of the original problem and its solution.

Remark 2. To get the solution of the undamped case $\sigma = 0$ one can use extrapolation methods.

Convergence

The convergence of the iteration depends on the magnitude of the perturbation function k_Δ^2. The more the periodicity is disturbed, the worse is the convergence. In the case of divergence one may help oneself by applying the following trick: Let $k_\Delta^2 = k_{\Delta,1}^2 + k_{\Delta,2}^2$, where $k_{\Delta,1}^2$ is small enough so that the problem $\Delta u + (k_{\text{per}}^2 + k_{\Delta,1}^2)(1 + \mathrm{i}\sigma)^2 u = f$ leads to a convergent iteration and is thus solvable with the above algorithm. By shifting the troubling term $k_{\Delta,2}^2(1+\mathrm{i}\sigma)^2 u$ to the right hand side one obtains again an iteration problem:

$$\Delta u_{n+1} + (k_{\text{per}}^2 + k_{\Delta,1}^2)(1 + \mathrm{i}\sigma)^2 u_{n+1} = f - k_{\Delta,2}^2(1 + \mathrm{i}\sigma)^2 u_n$$

This way one may reduce the problem recursively to solvable problems.

Perturbation of Multiple Cells

In the case $\Omega \not\subset C_0$ it is not necessary, to solve (15) on a larger lattice cell, since (13) and the left hand side of (15) remain unaffected. We only have to take into account more terms of the Bloch-Floquet transform of the right hand side of (15):

$$\tilde{f} \to \sum_{\mathbf{d} \in \Gamma_0} \tilde{f}(\mathbf{r} + \mathbf{d}) \exp(-\mathrm{i}\mathbf{k}_B \cdot \mathbf{d})$$

where $\Gamma_0 = \left\{ \mathbf{d} \in \Gamma \,|\, \operatorname{supp} \tilde{f} \cap (\mathbf{d} + C_0) \neq \emptyset \right\}$.

5 Examples

We implemented this algorithm for the one- and two-dimensional case. In the following we present a 1D as well as a 2D example. Figures 2 and 3 show the geometry of the 1D and 2D media which each consist of two materials with $k_1 = 6$ and $k_2 = 8$. The source term is $f(\mathbf{r}) = \exp(-25\mathbf{r} \cdot \mathbf{r})$ in Ω and $f = 0$ outside Ω, where $\Omega = [-0.5; 0.5]$ and $\Omega = [-0.5; 0.5]^2$, respectively. The damping parameter is in both cases $\sigma = 10^{-2}$.

Figure 4 shows the intensity $|u(\mathbf{r})|^2$ of the computed scattered field in the inner part of the infinite domain for the two-dimensional case.

6 Conclusions

Within the current work we demonstrated a dimensionally independent formulation for scattering problems with periodic exterior domains, that is valid for all kinds of infinite periodic structures with local defects. By means of a simple iterative scheme

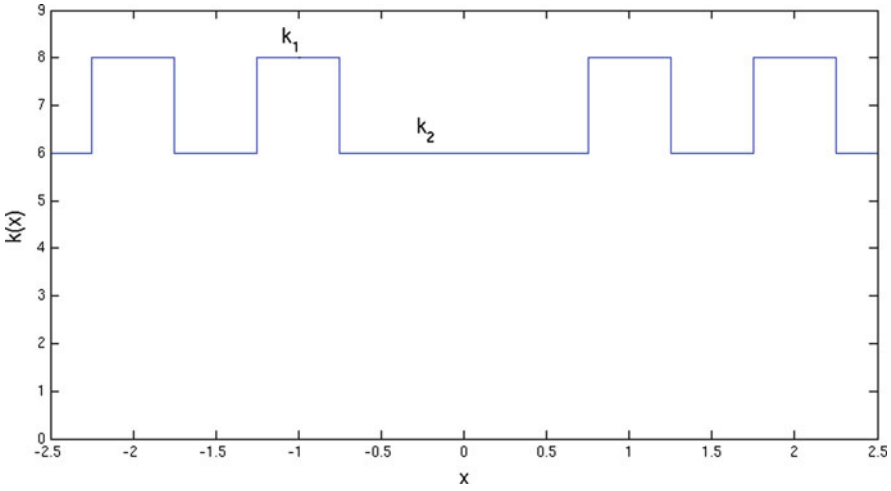

Fig. 2 1D geometry consisting of two materials with difference refractive indices

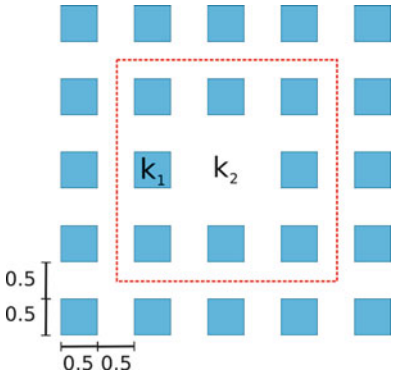

Fig. 3 2D geometry with square lattice. The red dashed line marks the domain which is depicted in Fig. 4

the original problem with local defects is reduced to a series of exact periodic problems which can be solved efficiently with standard numerical techniques. For each of the individual exact periodic subproblems the computational domain can be restricted to a finite region by applying the limiting absorption principle and the Bloch-Floquet transform. We demonstrated the feasibility of our formulation by implementing it for the one-dimensional as well as for the two-dimensional case. For both cases a practical test case has been shown to yield meaningful results with a good convergence behaviour (Fig. 5). Our investigations indicate that the convergence behaviour of the iteration depends on the magnitude of the perturbation. Consequently, for strongly perturbed geometries, the problem might not converge at all. However, for such cases, convergence can be re-established by employing a nested iteration.

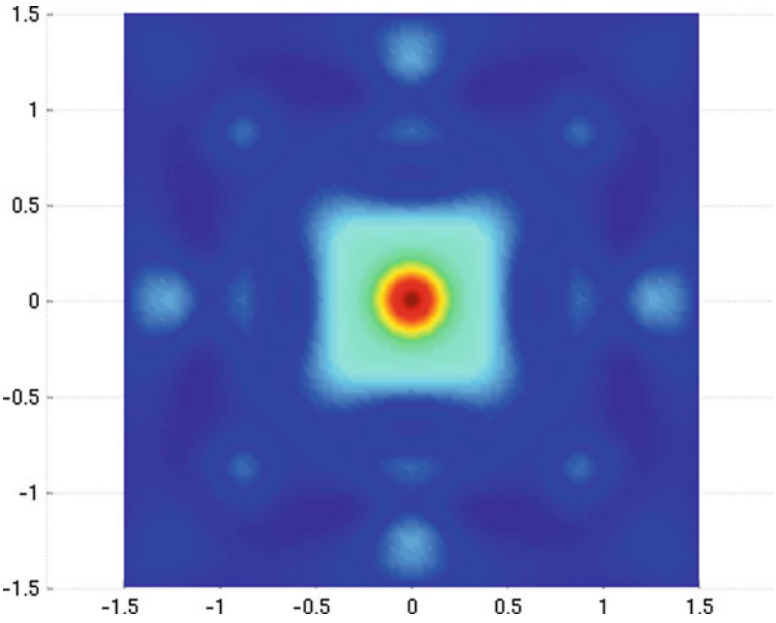

Fig. 4 Intensity of the computed 2d-solution for the infinite periodic scattering problem

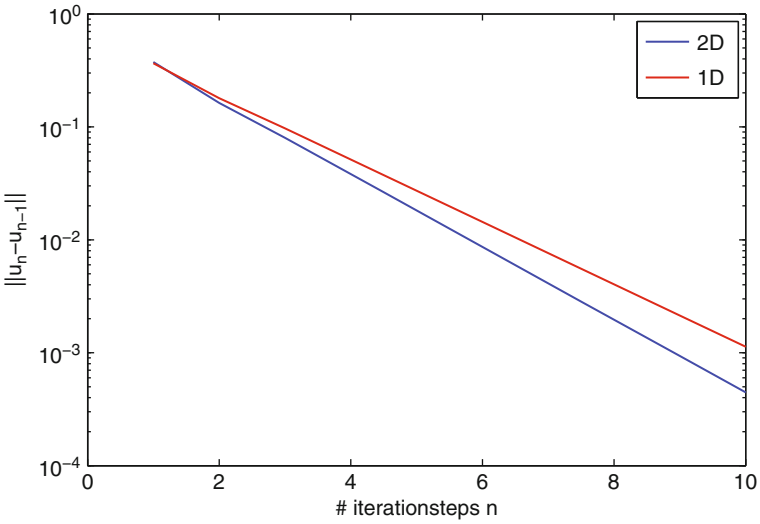

Fig. 5 Convergence of the iteration

References

1. Benisty, H., Berger, V., Gérard, J.M., Maystre, D., Tchelnokov, A.: Photonic Crystals. Towards Nanoscale Photonic Devices. Springer, Berlin (2008)
2. Botten, L.C., Dossou, K., Wilcox, S., McPhedran, R.C., de Sterke, C.M., Nicorovici, N.A., Asatryan, A.A.: Accurate defect mode modelling in photonic crystals using the generalised fictitious source superposition method. PIERS Online **3**(3), 320–324 (2007)
3. Fliss, S., Joly, P.: Exact boundary conditions for time-harmonic wave propagation in locally perturbed periodic media. Appl. Numer. Math. **59**, 2155–2178 (2009)
4. Joannopoulos, J.D., Johnson, S.G., Winn, J.N., Meade, R.D.: Photonic Crystals. Molding the Flow of Light. Princeton University Press, Princeton, NJ (2008)
5. Joly, P., Li, J., Fliss, S.: Exact boundary conditions for periodic waveguides containing a local perturbation. Comm. Comput. Phys. **1**(6), 945–973 (2006)
6. Kuchment, P.: The mathematics of photonic crystals. In: G. Bao, L. Cowsar, W. Masters (eds.) Mathematical Modeling in Optical Science, Frontiers in Applied Mathematics, vol. 22, pp. 207–272. SIAM, Philadelphia (2001)