Boundary Integral Representations in Photonic Crystals *

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1 Green's Identity

We start with the divergence theorem in $\mathbb{R}$. Let Ω_0 be a bounded domain with piecewise smooth boundary $\partial\Omega_0$ and $\mathbf{n}$, the unit outward vector normal to $\partial\Omega_0$. For a smooth field $w \in C^1(\bar{\Omega}_0)$,

$$\int_{\Omega_0} \nabla \cdot w dr = \int_{\partial\Omega_0} w \cdot n ds$$

Let $w = v\nabla u$, then

$$\nabla w = v\Delta u + \nabla v \cdot \nabla u.$$

By the divergence theorem,

$$\int_{\Omega_0} \nabla w dr = \int_{\Omega_0} (v\Delta u + \nabla v \cdot \nabla u) dr = \int_{\Omega_0} v\frac{\partial u}{\partial n} ds$$

Interchanging v and u, we have

$$\int_{\Omega_0} (u\Delta v + \nabla u \cdot \nabla v) dr = \int_{\Omega_0} u\frac{\partial v}{\partial n} ds$$

Thus we obtain the following *Green's Identity* by subtracting the above two identities:

$$\int_{\Omega_0} (u\Delta v - v\Delta u) dr = \int_{\Omega_0} (u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}) ds$$

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2 Boundary Integral Representation Using Green's Identity

In order to introducing Green functions, we first give an idea of the delta function $\delta(x)$, which satisfies

$$\delta(x) = \begin{cases} 0 & , \quad if \quad x \neq 0 \\ \infty & , \quad if \quad x = 0 \end{cases}$$

and

$$\int_{\mathbb{R}^n} \delta(x) = 1. \qquad \text{(unit point mass)}$$

The delta function has the following properties:

$$\int_{\mathbb{R}^n} \delta(x)\phi(x)dx = \phi(0)$$

and

$$\int_{\mathbb{R}^n} \delta(x - x_0)\phi(x)dx = \phi(x_0)$$

The second identity follows from $y = x - x_0$ and hence

$$\int_{\mathbb{R}^n} \delta(x - x_0)\phi(x)dx = \int_{\mathbb{R}^n} \delta(y)\phi(y + x_0)dy = \phi(x_0).$$

In the equation for the spatial factor of a time-harmonic acoustic wave

$$\nabla \cdot \tau \nabla u + \omega^2 \rho u = 0.$$

If τ is a constant in a domain Ω, we can write

$$\tau \nabla \cdot \nabla u + \omega^2 \rho u = 0,$$

or

$$\Delta u + k^2 u = 0, \quad where \quad k^2 = \frac{\omega^2 \rho}{\tau}$$

This is a *Helmholtz* equation. The Helmholtz equation in $\mathbb{R}^3$ admits a fundamental solution (Green function)

$$\Phi(\hat{r} - r) = \frac{1}{4\pi} \frac{e^{ik|\hat{r}-r|}}{|\hat{r} - r|}$$

i.e.

$$\Delta\Phi + k^2\Phi = \delta(\hat{r} - r)$$

In $\mathbb{R}^2$, it has a fundamental solution

$$\Phi(\hat{r} - r) = -\frac{i}{4}H_0^1(k_0|\hat{r} - r|),$$

where $H_0^1(z)$ is a Hankel function and $H_0^1(z) \sim \sqrt{\frac{2}{\pi z}}e^{i(z-\frac{\pi}{4})}$ as $z \to \infty$.

Suppose we have the Green function Φ. From the Green's identity, we have

$$\begin{aligned}\int_\Omega (u\Delta v - v\Delta u)dr &= \int_\Omega (u\Delta v + k^2uv - v\Delta u - k^2uv)dr \\ &= \int_\Omega (u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n})ds\end{aligned}$$

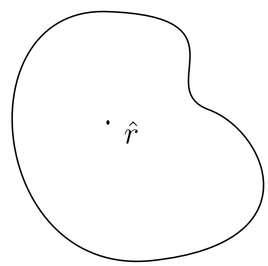

Figure 1: Case 1: $\hat{r}$ is in the interior.

Fix $\hat{r} \in \Omega$ and let $v = \Phi(\hat{r} - r)$, $u = u(r)$, then

$$\int_\Omega u(r)\delta(\hat{r} - r)dr = \int_\Omega \left[u(r)\frac{\partial\Phi(\hat{r} - r)}{\partial n(r)} - \Phi(\hat{r} - r)\frac{\partial u(r)}{\partial n(r)}\right] ds(r)$$

i.e.

$$u(\hat{r}) = \int_\Omega \left[u(r)\frac{\partial\Phi(\hat{r} - r)}{\partial n(r)} - \Phi(\hat{r} - r)\frac{\partial u(r)}{\partial n(r)}\right] ds(r)$$

However, if $\hat{r} \in \mathbb{R}^3 \setminus \bar{\Omega}$, we cannot take the same domain Ω to obtain similar expression, because $\Delta\Phi(\hat{r} - r) + k^2\Phi = 0$, i.e., the Green function does not have a singular point in Ω.

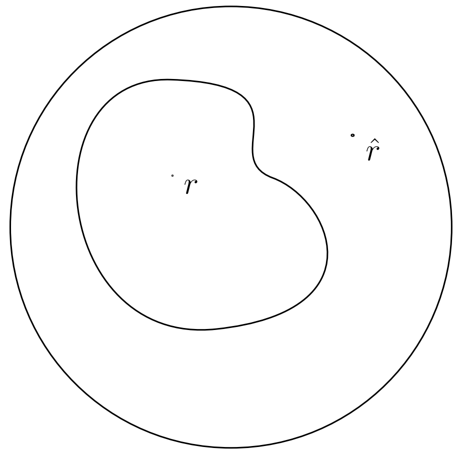

Figure 2: Case 2: $\hat{r}$ is in the exterior.

We fix this problem by taking an exterior domain $B_R \setminus \bar{\Omega}$, where B_R is a ball centered at $\hat{r}$ with radius R large enough, and so

$$u(\hat{r}) = \int_{\partial\Omega} \left[-u(r) \frac{\partial \Phi(\hat{r}-r)}{\partial n(r) + \Phi(\hat{r}-r)\frac{\partial u(r)}{\partial n(r)}} \right] ds(r) + \int_{\partial B_R} \left[u\frac{\partial \Phi}{\partial n} - \Phi \frac{\partial u}{\partial n} \right] ds(r)$$

The second integral vanishes if we assume the radiation conditions. One radiation condition is the Sommerfeld radiation condition:

$$\left(\frac{r}{|r|}, \nabla u(r) \right) - iku(r) = o\left(\frac{1}{|r|} \right), \quad as \quad |r| \to \infty.$$

The following theorem can be proved

Theorem 1 *Let $u \in \mathbb{R}^n \setminus \bar{\Omega}$ be a solution of the Helmholtz equation, $\Phi(\hat{r}, r)$ a fundamental solution. Assume they both satisfying the Sommerfeld radiation condition uniformly for all directions* $\mathbf{n}$. *Then*

$$\int_{\partial\Omega} \left[u(r)\frac{\Phi(\hat{r}, r)}{\partial n(r)} - \frac{\partial u(r)}{\partial n(r)}\Phi(\hat{r}, r) \right] ds(r) = u(\hat{r}), \qquad \hat{r} \in \mathbb{R} \setminus \bar{\Omega}$$

3 Periodic Structures and Associated Green Functions

Let us discuss the integral representation for photonic crystals. The structure we are interested in is a periodic media consisting of an array of rods with the same constant coefficients $\tau = \tau_1, \rho = \rho_1$ lying in a material with other same constant coefficients $\tau = \tau_0, \rho = \rho_0$. The spatial factor satisfies two equations

$$\Delta u + k_1^2 u = 0, \quad in \quad D \tag{1}$$
$$\Delta u + k_0^2 u = 0, \quad in \quad S \setminus \bar{D} \tag{2}$$

where $k_1^2 = \frac{\rho_1}{\tau_1}\omega^2$, $k_0^2 = \frac{\rho_0}{\tau_0}\omega^2$.

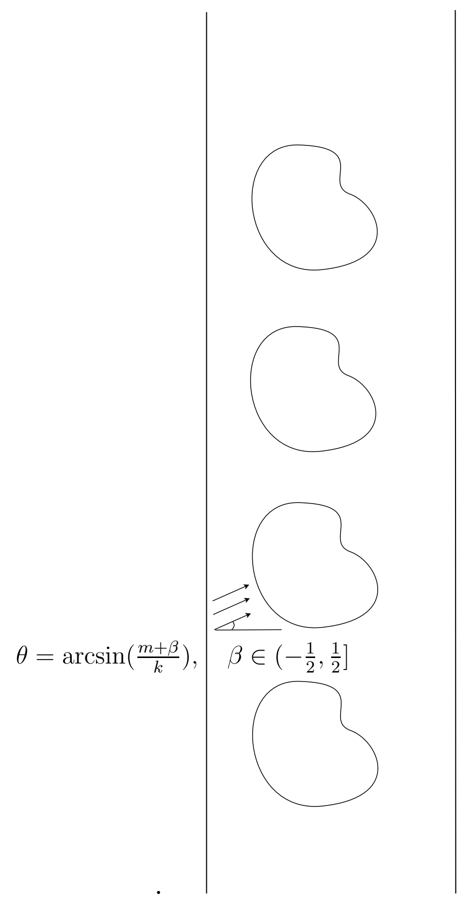

Figure 3: Periodic Structures and Incidental Waves.

The following matching conditions at the interfaces should be met

$$u_{int} = u_{ext} \tag{3}$$
$$\tau_1 \nabla u_{int} = \tau_0 \nabla u_{ext}, \tag{4}$$

or

$$\nabla u_{int} = \frac{\tau_0}{\tau_1}\nabla u_{ext} = \nu \nabla u_{ext}.$$

Suppose an incident field is produced at an angle of θ to the $x-$axis, and has the form

$$u_{inc} = e^{i\sqrt{k^2-(m+\beta)^2}x+i(m_\beta)y}.$$

It satisfies the Helmholtz equation and the pseudoperiodicity $u(x, y+2\pi) = u(x,y)e^{i\beta 2\pi}$.

We now consider a pseudoperiodic scattered field u_{sc} that satisfies a radiation condition at $x = \pm\infty$.

We assume $k^2-(m+\beta)^2 \neq 0$. Let μ_m be defined by $\mu_m^2-(m+\beta)^2+k^2 = 0$, (or $\mu_m^2 = (m+\beta)^2 - k^2$). The series $\Phi(r) = -\frac{1}{4\pi}\sum_{m=-\infty}^{\infty} \frac{1}{i\mu_m} e^{i\mu_m|x|+i(m+\beta)y}$ converges and

$$\Delta\Phi + k^2\Phi = -\sum_{m=-\infty}^{\infty} \delta(x, y-2\pi n)e^{2\pi n i\beta}.$$

This function is pseudoperiodic

$$\Phi(x, y+2\pi) = \Phi(x,y)e^{i2\pi\beta}.$$

In order to ensure the radiation condition, we make the following sign determination:

- If $\mu_m^2 < 0$, $\sqrt{|\mu_m|^2} = \eta_m$, then we take $\mu_m = \eta_m i$.
- If $\mu_m^2 > 0$, $\eta_m = |\mu_m|$, then we take $\mu_m > 0$.

The first case corresponds to exponentially decaying harmonics; the second gives outwardly propagating harmonics.

Notice that for our choices of Green functions in this section, there is a negative sign besides δ in contrast to the previous section. So the Green's identity implies that, for a bounded domain and a Helmholtz field u,

$$u(\hat{r}) + \int_{\partial\Omega} \left[\frac{\partial\Phi(\hat{r}-r)}{\partial n(r)}u(r) - \Phi(\hat{r}-r)\frac{\partial u(r)}{\partial n(r)}\right] ds(r) = 0.$$

4 Boundary Integral Representations for Periodic Structures

Now we compute u in terms of the boundary integrals for both interior and exteriors.

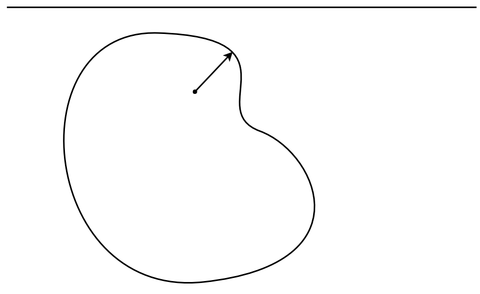

Figure 4: In the interior, let $h \to 0$

For $\hat{r} \in \partial D$ and $h > 0$,

$$u_{int}(\hat{r}-hn(\hat{r}))+\int_{\partial\Omega}\left[\frac{\partial\Phi(\hat{r}-hn(\hat{r})-r)}{\partial n(r)}u_{int}(r)-\Phi(\hat{r}-hn(\hat{r})-r)\frac{\partial u_{int}(r)}{\partial n(r)}\right]ds(r)=0. \tag{5}$$

Let $h \to 0$, then the term $\frac{\partial\Phi}{\partial n}$ produces a singular contribution

$$\lim_{h\to 0}\int_{\partial D}\frac{\partial\Phi(\hat{r}-hn(\hat{r})-r)}{\partial n(r)}u_{int}(r)ds(r)=-\frac{1}{2}u_{int}(\hat{r})+\int_{\partial D}\frac{\partial\Phi(\hat{r}-r)}{\partial n(r)}u_{int}(r)ds(r), \quad \hat{r}\in\partial D.$$

So for $\hat{r} \in \partial D$, $u_{int}(\hat{r})$ satisfies the integral equation

$$\frac{1}{2}u_{int}(\hat{r})+\int_{\partial D}\left[\frac{\partial\Phi(\hat{r}-r)}{\partial n(r)}u_{int}(r)-\Phi(\hat{r}-r)\frac{\partial u_{int}}{\partial n(r)}(r)\right]ds(r)=0.$$

By the matching conditions, we obtain

$$\frac{1}{2}u_{ext}(\hat{r})+\int_{\partial D}\left[\frac{\partial\Phi}{\partial n}u_{ext}-\Phi\frac{\partial u_{ext}}{\partial n}\right]ds=0 \tag{6}$$

The exterior is a bit more complicated. For $\hat{r}+hn(\hat{r}) \in S \setminus \bar{D}$,

$$u_{ext}(\hat{r}+hn(\hat{r}))+\int_{\Gamma\setminus\partial D}\left[\frac{\partial\Phi(\hat{r}+hn(\hat{r})-r)}{\partial n(r)}u_{ext}(r)-\Phi(\hat{r}+hn(\hat{r})-r)\frac{\partial u_{ext}(r)}{\partial n(r)}\right]ds(r)=0 \tag{7}$$

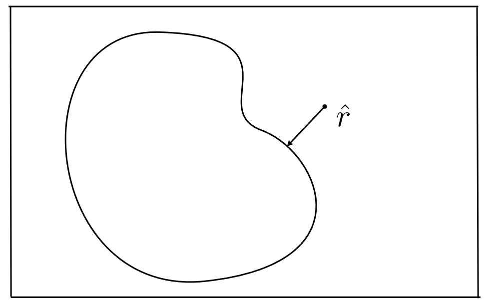

Figure 5: In the exterior, let $h \to 0$

By the radiation condition of u_{sc}, we know

$$\int_\Gamma \left[\frac{\partial \Phi}{\partial n} u_{sc} - \Phi \frac{\partial u_{sc}}{\partial n}\right] ds = 0.$$

So the integral of u_{ext} on Γ,

$$\begin{aligned}\int_\Gamma \left[\frac{\partial \Phi}{\partial n} u_{ext} - \Phi \frac{\partial u_{ext}}{\partial n}\right] ds &= \int_\Gamma \left[\frac{\partial \Phi}{\partial n} u_{inc} - \Phi \frac{\partial u_{inc}}{\partial n}\right] + \int_\Gamma \left[\frac{\partial \Phi}{\partial n} u_{sc} - \Phi \frac{\partial u_{sc}}{\partial n}\right] \\ &= \int_\Gamma \left[\frac{\partial \Phi}{\partial n} u_{inc} - \Phi \frac{\partial u_{inc}}{\partial n}\right] ds \\ &= -u_{int}(\hat{r} + hn(\hat{r})).\end{aligned}$$

Substitute it into (6), then we get

$$\begin{aligned}u_{ext}(\hat{r} + hn(\hat{r})) + \int_{\partial D} \Bigg[&-\frac{\partial \Phi(\hat{r} + hn(\hat{r}) - r)}{\partial n(r)} u_{ext}(r) \\ &+ \Phi(\hat{r} + hn(\hat{r}) - r)\frac{\partial u_{ext}(r)}{\partial n(r)}\Bigg] ds(r + hn(\hat{r})) \\ = u_{inc}(\hat{r} + hn(\hat{r})).\end{aligned} \tag{8}$$

Let $h \to 0$ from the exterior, the since the term $\frac{\partial \Phi}{\partial n}$ produces a singular contribution

$$\lim_{h\to 0}\int_{\partial D} -\frac{\partial \Phi(\hat{r} + hn(\hat{r}) - r)}{\partial n(r)} u_{ext}(r) ds(r) = -\frac{1}{2}u_{ext}(\hat{r}) + \int_{\partial D} -\frac{\partial \Phi(\hat{r})}{\partial n(r)} u_{ext}(r) ds(r), \quad \hat{r} \in \partial D.$$

we have

$$\frac{1}{2}u_{ext}(\hat{r}) + \int_{\partial D} \left[-\frac{\partial \Phi(\hat{r} - r)}{\partial n(r)} u_{ext}(r) + \Phi(\hat{r} - r)\frac{\partial u_{ext}(r)}{\partial n(r)}\right] ds(r) = u_{inc}(\hat{r}). \tag{9}$$

The two equations (6) (9) form a system of $u_{ext}(\hat{r})$ and $\frac{\partial u_{ext}}{\partial n}(\hat{r})$.

5 Numerical Computation

To solve the system numerically, we choose a finite number of sample points $\{\hat{r}_j\}_{j=1}^N$ on ∂D and approximate all the functions in the system by their linear interpolations at these sample points, and we also apprimate the integrals by the integral of the linear interpolations. Or equivalently, in the language of function spaces, we approximate $u_{ext(\hat{r})}$ and $\frac{\partial u_{ext}}{\partial n}(\hat{r})$ by a linear combination of linearly independent basis functions $\{h_i\}_{i=1}^N$ on $C(\partial D)$:

$$u_{ext}(\hat{r}) = \sum_{i=1}^N a_i h_i(\hat{r}), \quad \hat{r} \in \partial D \tag{10}$$

$$\frac{\partial u_{ext}}{\partial n}(\hat{r}) = \sum_{i=1}^N b_i h_i(\hat{r}) \tag{11}$$

Denote

$$L_1(u, \frac{\partial u}{\partial n})(\hat{r}) = \frac{1}{2}u(\hat{r}) + \int_{\partial D} \left[-\frac{\partial \Phi(\hat{r}-r)}{\partial n(r)} u_{ext}(r) + \Phi(\hat{r}-r)\frac{\partial u_{ext}(r)}{\partial n(r)} \right] ds(r)$$
$$L_2(u, \frac{\partial u}{\partial n})(\hat{r}) = \frac{1}{2}u(\hat{r}) + \int_{\partial D} \left[\frac{\partial \Phi(\hat{r}-r)}{\partial n(r)} u_{ext}(r) - \nu\Phi(\hat{r}-r)\frac{\partial u_{ext}(r)}{\partial n(r)} \right] ds(r)$$

We get an approximating finite-dimensional linear system

$$L_1(\sum a_i h_i, \sum b_i h_i)(\hat{r}_j) = u_{inc}(\hat{r}_j), \quad j = 1, \dots, N$$
$$L_2(\sum a_i h_i, \sum b_i h_i)(\hat{r}_j) = 0, \quad j = 1, \dots, N$$

This is a $2N \times 2N$ linear system for $\{a_i, b_i\}_{j=1}^N$.

The values of u in D and in $S \setminus \bar{D}$ can be obtained by (5) and (8) using similar discretization.

6 Further Readings

The proof of the Theorem can be found in Theorem 3.3 in [1]. The singular contribution of the double-layer potential is calculated in Theorem 2.13 in

[1]. A general definition of the integral representations is given in [3]. In [2], some numerical computations are implemented for a system related to the system mentioned here.

References

[1] D.Colton and R.Kress, *Integral Equation Methods in Scattering Theory*, Wiley- Interscience, 1983, Russian translation 1987.

[2] M. Haider, S. Shipman, and S. Venakides, *Boundary-Integral Calculations of Two-Dimensional Electromagnetic Scattering in Infinite Photonic Crystal Slabs: Channel Defects and Resonances*, SIAM J. Appl. Math., Vol. 62 (2002), No. 6, pp. 2129-2148.

[3] S. Shipman and S. Venakides, *Resonance and Bound States in Photonic Crystal Slabs*, SIAM J. Appl. Math., Vol. 64, No. 1 (2003), pp. 322-342.