Outgoing Wave Conditions in Photonic Crystals and Transmission Properties at Interfaces

Workshop: “Waves in periodic media and metamaterials”

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Fermat’s principle of the fastest path:

Light finds the fastest way to reach the destination!

\[
\frac{\sin \Theta_1}{\sin \Theta_2} = \frac{v_1}{v_2} = \frac{n_2}{n_1}
\]
Geometric optics vs. Wave equation

Fermat’s principle of the fastest path:
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\[
\frac{\sin \Theta_1}{\sin \Theta_2} = \frac{v_1}{v_2} = \frac{n_2}{n_1}
\]

Huygens’ principle of superpositions
Wave equation

\[
\partial_t^2 u = \Delta u
\]

Numerical solution
# Maxwell’s equations and negative index

## Maxwell’s Equations (1865)

\[
\begin{align*}
\text{curl } E &= i\omega \mu H \\
\text{curl } H &= -i\omega \varepsilon E
\end{align*}
\]

- \(E\): electric field, \(H\): magnetic field
- \(H, E \sim e^{-i\omega t}\)

- \(\text{Re } \varepsilon < 0\) possible
- \(\mu\) is always 1
- \(\text{Re } \mu \varepsilon < 0\): medium is opaque

## Veselago (1968)

Materials with negative index

\(\varepsilon < 0\) and \(\mu < 0 \Rightarrow\) negative index!

## Pendry et al. (~ 2000)

Design of a negative index meta-material

Use split rings and wires
The material parameter $\varepsilon_\eta$ is

$$
\varepsilon_\eta = \begin{cases} 
1 + i \frac{\kappa}{\eta^3} & \text{in the rings} \\
1 & \text{else}
\end{cases}
$$

Effective coefficients $\mu_{\text{eff}}$ and $\varepsilon_{\text{eff}}$.

The parameter $\eta$ appears $4 \times$:

1. size of the microstructure ($\eta$)
2. thin rings ($2\beta\eta^2$)
3. very thin slit ($2\alpha\eta^4$)
4. high conductivity ($\kappa\eta^{-3}$)
Microscopic geometry with wires

\[(H^n, E^n)\) solves Maxwell, \((H^n, E^n) \to (\hat{H}, \hat{E})\) “geometrically”


\[
curl \hat{E} = i\omega \mu_{\text{eff}} \hat{H}
\]

\[
curl \hat{H} = -i\omega \varepsilon_{\text{eff}} \hat{E}
\]

with negative (for appropriate geometry and \(\text{Re}(\varepsilon_w) < 0\)) coefficients

\[
\mu_{\text{eff}} = \mu_{\text{eff,R}} = (\hat{M})^{-1} \quad \text{and} \quad \varepsilon_{\text{eff}} = \varepsilon_{\text{eff,R}} + \pi \gamma^2 \varepsilon_W.
\]
Our question:

Is this refraction at a negative index material?

Image taken from:

An interesting observation about wave transmission

Our question:

Is this refraction at a negative index material?

Explanation of the effect in [LJJP]:
The solution in the photonic crystal is a Bloch wave, determined by two facts:

- it has the right frequency
- it conserves the vertical wave number

Together, this can explain negative refraction

Image taken from

Mathematical subject: **Radiation condition in periodic media**

- Homogenous media (Sommerfeld, 1912)
- Periodic media (Fliss and Joly, ARMA 2016)
- Periodic media with an interface (Lamacz and S., 2016)
Homogeneous problem \(-\Delta u = \omega^2 u\) in \(\mathbb{R}^n\)

**Fundamental solutions**

Two fundamental Helmholtz solutions for \(x \in \mathbb{R}^3\):

\[
\begin{align*}
 u_{\text{out}}(x) &:= \frac{1}{|x|} e^{i\omega |x|} \quad \text{and} \quad u_{\text{in}}(x) := \frac{1}{|x|} e^{-i\omega |x|}
\end{align*}
\]

Time-dependence \(e^{-i\omega t}\) implies: \(u_{\text{out}}\) is an outgoing wave, \(u_{\text{in}}\) an incoming wave.

**Sommerfeld condition**

\[
|x|^{(n-1)/2}(\partial_{|x|} u - i\omega u)(x) \rightarrow 0 \quad \text{as} \quad |x| \rightarrow \infty \tag{1}
\]

Both elementary solutions decay for \(|x| \rightarrow \infty\). It is not reasonable to demand only a decay property.

- \(u_{\text{out}}\) satisfies (1), it is admissible
- \(u_{\text{in}}\) does not satisfy (1), it is not admissible

**Justification (Sommerfeld):** Radiation condition implies uniqueness
**Radiation in a periodic wave-guide: Fliss and Joly, 2016**

The periodic waveguide is
- **neither** 2-dimensional (no decay of waves)
- **nor** 1-dimensional (variations in vertical direction)

**Idea:** The solution consists of finitely many outgoing Bloch waves at $+\infty$

**Definition (Outgoing radiation condition, Fliss and Joly, 2016)**

A function $u$ solves the outgoing radiation condition to the right if

$$u(. + (p, 0)) = \sum_{m=1}^{N(\omega)} u_m^+ \Phi_m e^{ip\xi_m^+} + w^+. (. + (p, 0)), \quad (2)$$

where $w^+$ has exponential decay at $+\infty$.

**Justification:** Radiation condition implies existence and uniqueness
The geometry of the transmission problem. We are interested in waves that are generated in the photonic crystal.

\[-\nabla \cdot (a \nabla u) = \omega^2 u\]

Program:

1. Develop an “outgoing wave condition” in a photonic crystal
2. Derive a uniqueness result (justification of the condition)
3. Conclude properties of transmitted waves
Bloch expansion (… on one page!)

1.) $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is written with a Fourier transform:

$$f(x) = \int_{\mathbb{R}^n} \hat{f}(\xi) e^{2\pi i \xi \cdot x} d\xi$$
Negative refraction
Radiation conditions
Uniqueness and transmission properties

Known radiation conditions
Bloch wave analysis
Outgoing wave condition

Bloch expansion (… on one page!)

1.) \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) is written with a Fourier transform:

\[
f(x) = \int_{\mathbb{R}^n} \hat{f}(\xi) e^{2\pi i \xi \cdot x} \, d\xi
\]

2.) \( \xi \) is written as \( \xi = k + j \) with \( k \in \mathbb{Z}^n \) and \( j \in [0, 1)^n =: Z \)

\[
f(x) = \int_{Z} \sum_{k} \hat{f}(k + j) e^{2\pi i k \cdot x} e^{2\pi i j \cdot x} \, dj
\]

\[
=: F
\]
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$$f(x) = \int_Z \sum_k \hat{f}(k + j) e^{2\pi i k \cdot x} e^{2\pi i j \cdot x} \, dj$$

3.) Periodic $F = F(x; j)$ is expanded in periodic eigenfunctions $\Psi_{j,m}(x)$:

$$F(x; j) = \sum_{m \in \mathbb{N}} \alpha_{j,m} \Psi_{j,m}(x)$$

Periodic $F = F(x; j)$ is expanded in periodic eigenfunctions $\Psi_{j,m}(x)$:

$$U_{j,m}(x) := \Psi_{j,m}(x) e^{2\pi i j \cdot x}$$ solves

$$-\nabla \cdot (a(x) \nabla U_{j,m}(x)) = \mu_{j,m} U_{j,m}(x)$$
1.) $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is written with a Fourier transform:

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3.) Periodic $F = F(x; j)$ is expanded in periodic eigenfunctions $\Psi_{j,m}(x)$:

$$F(x; j) = \sum_{m \in \mathbb{N}} \alpha_{j,m} \Psi_{j,m}(x)$$

$$U_{j,m}(x) := \Psi_{j,m}(x) e^{2\pi i j \cdot x} \text{ solves } -\nabla \cdot (a(x) \nabla U_{j,m}(x)) = \mu_{j,m} U_{j,m}(x)$$

Result: The operator $\mathcal{L}_0 = -\nabla \cdot (a(\cdot) \nabla)$ acts as a multiplier:

$$f(x) = \int_{Z} \sum_{m \in \mathbb{N}} \alpha_{j,m} U_{j,m}(x) \, dj, \quad \mathcal{L}_0 f = \int_{Z} \sum_{m \in \mathbb{N}} \alpha_{j,m} \mu_{j,m} U_{j,m}(x) \, dj$$
Expansion of solutions

We consider \( u \) only on the marked square

After a shift:
\( u \in L^2((0, R\varepsilon) \times (0, R\varepsilon)) \)

Wave-vector: \( j \in \mathbb{Z} := [0, 1)^2 \). Eigenvalue number: \( m \in \mathbb{N}_0 \)
Multiindex: \( \lambda = (j, m) \in I_K \). Basis: \( U^+_\lambda(x) := \Psi^+_\lambda(x) e^{2\pi i \theta(\lambda) \cdot x / \varepsilon} \)

Expansion of an arbitrary function \( u \) in Bloch waves

\[
 u(x) = \sum_{\lambda \in I_K} \alpha^+_\lambda U^+_\lambda(x)
\]

Idea: For “outgoing solutions” we demand:

- \( u \) (on the right) consists only of right-going Bloch modes

Note: \( u \) periodic \( \rightarrow \) Bloch expansion is a sum
In the expansion
\[ u(x) = \sum_{\lambda \in I_K} \alpha_\lambda^+ U_\lambda^+(x) \]
which Bloch modes are outgoing?

**Recall:** The Poynting vector \( P := E \times H \) measures the energy flux.

**Poynting number**

For \( \lambda \in I \), the Poynting number \( P_\lambda^+ \) describes the right-going energy:

\[ P_\lambda^+ := \text{Im} \int_{Y_\varepsilon} \overline{U_\lambda^+(x)} e_1 \cdot \left[ a^\varepsilon(x) \nabla U_\lambda^+(x) \right] \, dx \]

**Index sets:** Left-going waves and “vertical waves”

\[ I_{<0}^+ := \{ \lambda \in I \mid P_\lambda^+ < 0 \} \quad \text{and} \quad I_{=0}^+ := \{ \lambda \in I \mid P_\lambda^+ = 0 \} \]

**Projection:** Onto left-going waves

\[ \Pi_{<0}^+ u(x) := \sum_{\lambda \in I_K \cap I_{<0}^+} \alpha_\lambda^+ U_\lambda^+(x) \]
Given $u$ on $\mathbb{R} \times (0, h)$, height $h = \varepsilon K$, factor $R \in KN$

**Large square:** $RY_\varepsilon = (0, R\varepsilon) \times (0, R\varepsilon)$

$\tilde{u} : \mathbb{R}^2 \to \mathbb{C}$ the $h$-periodic vertical extension

Define $u_R^+ : RY_\varepsilon \to \mathbb{C}$ by

$$u_R^+(x_1, x_2) := \tilde{u}(R\varepsilon + x_1, x_2)$$

Expand $u_R^+$:

$$u_R^+(x) = \sum_{\lambda \in I_R} \alpha_{\lambda, R}^+ U_\lambda^+(x)$$

The coefficients $(\alpha_{\lambda, R}^+)_{\lambda \in I}$ encode the behavior of $u$ for large $x_1$
Outgoing wave condition

Given \( u \) on \( \mathbb{R} \times (0, h) \), height \( h = \varepsilon K \), factor \( R \in K \mathbb{N} \)

**Large square:** \( RY_\varepsilon = (0, R\varepsilon) \times (0, R\varepsilon) \)

\( \tilde{u} : \mathbb{R}^2 \to \mathbb{C} \) the \( h \)-periodic vertical extension

Define \( u^+_R : RY_\varepsilon \to \mathbb{C} \) by

\[
 u^+_R(x_1, x_2) := \tilde{u}(R\varepsilon + x_1, x_2)
\]

Expand \( u^+_R \):

\[
 u^+_R(x) = \sum_{\lambda \in I_R} \alpha^+_{\lambda, R} U^+_\lambda(x)
\]

The coefficients \( (\alpha^+_{\lambda, R})_{\lambda \in I} \) encode the behavior of \( u \) for large \( x_1 \)

**Definition (Outgoing wave condition)**

We say that \( u \) satisfies the outgoing wave condition on the right if:

a) \( \int_0^h \int_L^{L+1} |u|^2 \) is bounded, independently of \( L \geq 0 \), and

b) \[
 \int_{RY_\varepsilon} |\Pi^+_{<0}(u^+_R)|^2 \to 0 \text{ as } R \to \infty
\]
Transmission problem

- \( a \) constant on the left, periodic on the right

Helmholtz equation: \(-\nabla \cdot (a \nabla u) = \omega^2 u\), periodic in vertical direction

Outgoing wave conditions, on the right:

\[
\int_{RY}^{\infty} |\Pi_{<0}^+ (u_R^+)|^2 \to 0 \text{ as } R \to \infty
\]

**Wishful thinking:** For every frequency \( \omega > 0 \)

- There exists a solution to the problem
- The solution to the problem is unique
Our wish-list

Transmission problem

*a* constant on the left, periodic on the right

Helmholtz equation: \(-\nabla \cdot (a\nabla u) = \omega^2 u\), periodic in vertical direction

Outgoing wave conditions, on the right:

\[
\int_{R_{Y\varepsilon}} \left| \Pi_{<0}^+ (u_R^+) \right|^2 \to 0 \text{ as } R \to \infty
\]

Wishful thinking: For every frequency \(\omega > 0\)

- There exists a solution to the problem
- The solution to the problem is unique

Uniqueness cannot be expected

There are surface-waves \(\longrightarrow\) no uniqueness!
Let $u_R \in L^2(W_R; \mathbb{C})$ be a sequence

$$u_R(x) = \sum_{\lambda \in I_R} \alpha^\pm_{\lambda} U^\pm_{\lambda}(x)$$

Discrete Bloch-measure for fixed $l \in \mathbb{N}_0$:

$$\nu^\pm_{l,R} := \sum_{\lambda = (j,l) \in I_R} |\alpha^\pm_{\lambda}|^2 \delta_j$$

where $\delta_j$ denotes the Dirac measure in $j \in \mathbb{Z}$. If, as $R \to \infty$,

$$\nu^\pm_{l,R} \to \nu^\pm_{l,\infty}$$

in the sense of measures, then

$$\nu^\pm_{l,\infty} \in \mathcal{M}(\mathbb{Z})$$

is a Bloch measure generated by $u$. 

The Brillouin zone $Z = [0, 1)^2$. A periodic $u$ is expanded with discrete values of $j \in \mathbb{Z}$. 

Frequency assumption with Bloch-eigenvalues $\mu_{m}^{\pm}(j)$:

$$\omega^2 < \inf_{j \in \mathbb{Z}, m \geq 1} \mu_{m}^{+}(j)$$

**Theorem (Uniqueness)**

Let $u$ and $\tilde{u}$ be two solutions of the transmission problem and let $v := u - \tilde{u}$ be the difference. Then:

- the Bloch measure of $v$ is supported on vertical waves
- for non-singular frequencies $\omega$: the Bloch measure of $v$ vanishes

**Interpretation of the result:**

Waves must be localized to the interface

For general $\omega$: vertical waves are possible

**Figure:** The indices $j \in \mathbb{Z}$ corresponding to “vertical waves”
Uniqueness follows from energy conservation

Poynting vector bilinear form $b_R^\pm : L^2(W_R; \mathbb{C}) \times H^1(W_R; \mathbb{C}) \to \mathbb{C}$:

$$b_R^+(u, v) := \int_{W_R} \bar{u}(x) e_1 \cdot [a(x) \nabla v(x)] \, dx$$

Let $v$ solve the Helmholtz equation with coefficients $a$, use

$$\vartheta(x) := \begin{cases} 
1 & \text{if } |x_1| \leq \varepsilon R \\
2 - \frac{|x_1|}{\varepsilon R} & \text{if } \varepsilon R < |x_1| < 2\varepsilon R \\
0 & \text{if } |x_1| \geq 2\varepsilon R 
\end{cases}$$

and the test-function $\vartheta(x) \overline{v}(x)$:

$$\int_{\mathbb{R}} \int_0^h \left\{ a \vartheta |\nabla v|^2 + a \partial_{x_1} \vartheta \overline{v} \partial_{x_1} v \right\} = \omega^2 \int_{\mathbb{R}} \int_0^h \vartheta |v|^2$$

Take the imaginary parts and obtain the energy conservation

$$\text{Im} b_R^- (v_R^-, v_R^-) = \text{Im} b_R^+ (v_R^+, v_R^+)$$

**Result:** If both terms have opposite sign, they must vanish!
Show $\nu_{l,\infty}^\pm = 0$ for $l \geq 1$

Let $\delta > 0$ be a number with $\delta \leq |\omega^2 - \mu_{(j,l)}|^2$ for all $j$ and $l \geq 1$. Then, formally,

$$\delta \int_{W_R} \left| \Pi_{l \geq 1}^{ev, +}(u_R^+) \right|^2 = \delta \sum_{\lambda = (j,l) \in I_R, l \geq 1} \left| \langle u_R^+, U_\lambda \rangle_R \right|^2$$

$$\leq \sum_{\lambda = (j,l) \in I_R, l \geq 1} \left| (\omega^2 - \mu_\lambda) \langle u_R^+, U_\lambda \rangle_R \right|^2$$

$$\leq \sum_{\lambda \in I_R} \left| \langle \omega^2 u_R^+, U_\lambda \rangle_R - \langle \mu_\lambda u_R^+, U_\lambda \rangle_R \right|^2$$

$$\overset{(*)}{=} \sum_{\lambda \in I_R} \left| \langle \mathcal{L}_0(u_R^+), U_\lambda \rangle_R - \langle \mu_\lambda u_R^+, U_\lambda \rangle_R \right|^2 = 0$$

The calculation can be made precise with cut-off functions on large squares. Result for Bloch measure: $\nu_{l,\infty}^\pm = 0$ for $l \geq 1$

Similar calculations yield:

$\text{supp}(\nu_{0,\infty}^\pm) \subset \{ j \in \mathbb{Z} | \mu_{0}^\pm(j) = \omega^2, j_2 \in \mathbb{N}/K \}$
Transmission condition

Assume again: Frequency below second band
The vertical wave number is conserved:

**Theorem (Transmission conditions)**

*Let $u$ be a solution of the transmission problem. Let $\nu_{l,\infty}^{\pm}$ be a Bloch measure to $u$. Then: $\nu_{l,\infty}^{\pm} = 0$ for $l \geq 1$. For $l = 0$ holds*

\[
\text{supp}(\nu_{0,\infty}^{\pm}) \subset \{ j \in \mathbb{Z} \mid \mu_0^{\pm}(j) = \omega^2, j_2 \in \mathbb{N}/K \}
\]

*and*

\[
\text{supp}(\nu_{0,\infty}^{\pm}) \subset \{ j \in \mathbb{Z} \mid j_2 = k_2 \} \cup J_{\pm,0,0}^{\pm}
\]

Waves must have:
- the correct energy
- the correct $k_2$ (or be vertical)

The theorem follows from uniqueness: Compare $u$ with its projection to the vertical wave number $k_2$. 
Conclusions and open problems

**Corollary:** For non-singular frequencies $\omega$, the Bloch measure of $u$ is supported on $\{ j \in \mathbb{Z} \mid j^2 = k^2 \}$.

$\longrightarrow$ conservation of the vertical wave number

Negative refraction can therefore be explained ...

... using that the vertical wave number is conserved.

**Open for the transmission problem:**

1. Existence with limiting absorption?
2. Vertical waves excluded?
3. Implementation of the outgoing wave condition?
Conclusions and open problems

**Corollary:** For non-singular frequencies $\omega$, the Bloch measure of $u$ is supported on \( \{j \in \mathbb{Z} \mid j^2 = k^2\} \).

\[ \rightarrow \quad \text{conservation of the vertical wave number} \]

Negative refraction can therefore be explained …

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**Open for the transmission problem:**

1. Existence with limiting absorption?
2. Vertical waves excluded?
3. Implementation of the outgoing wave condition?

Thank you!