Outgoing Wave Conditions in Photonic Crystals and Transmission Properties at Interfaces

Workshop: "Waves in periodic media and metamaterials"

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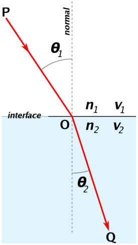
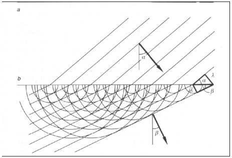
Geometric optics vs. Wave equation

Fermat's principle of **the fastest path:**

Light finds the fastest way to reach the destination!

$$\frac{\sin \Theta_1}{\sin \Theta_2} = \frac{v_1}{v_2} = \frac{n_2}{n_1}$$

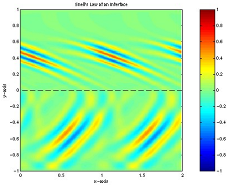




Huygens' principle of **superpositions**

Wave equation

$$\partial_t^2 u = \Delta u$$



Numerical solution

Maxwell's equations and negatve index

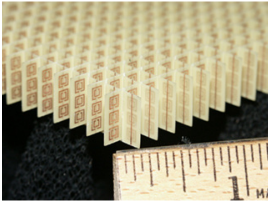
Maxwell's Equations (1865)

$$\begin{aligned} \operatorname{curl} E &= i\omega\mu H \\ \operatorname{curl} H &= -i\omega\varepsilon E \end{aligned}$$

E: electric field, H: magnetic field

$$H, E \sim e^{-i\omega t}$$

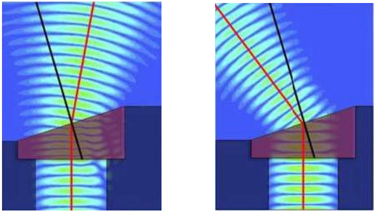
- $\operatorname{Re}\varepsilon < 0$ possible
- μ is always 1
- $\operatorname{Re}\mu\varepsilon < 0$: medium is opaque



Veselago (1968)

Materials with negative index

$\varepsilon < 0$ and $\mu < 0 \Rightarrow$ negative index!

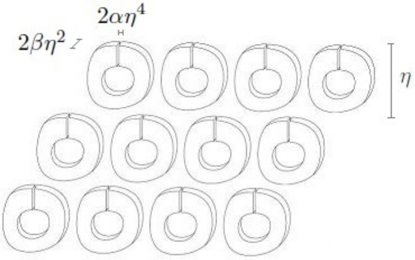


Solutions for positive and negative index

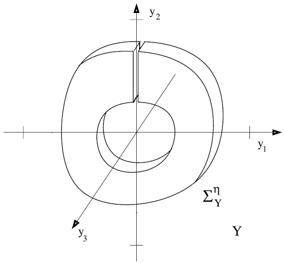
Pendry et al. ($\sim$ 2000)

Design of a negative index meta-material
Use split rings and wires

Microscopic split-ring geometry



$$\Sigma_\eta := \bigcup_k \eta(k + \Sigma_Y^\eta)$$



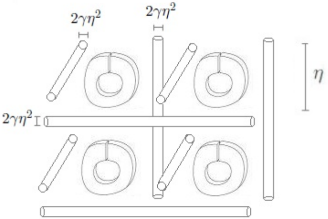
The material parameter ε_η is

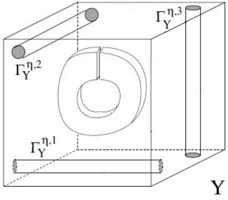
$$\varepsilon_\eta = \begin{cases} 1 + i\dfrac{\kappa}{\eta^3} & \text{in the rings} \\ 1 & \text{else} \end{cases}$$

The parameter η appears $4\times$:

1. size of the microstructure (η)
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^η, E^η) solves Maxwell, $(H^\eta, E^\eta) \to (\hat{H}, \hat{E})$ *"geometrically"*

Effective Maxwell system (A.Lamacz & B.S., 2016)

$$\operatorname{curl} \hat{E} = i\omega\mu_{\text{eff}}\, \hat{H}$$
$$\operatorname{curl} \hat{H} = -i\omega\varepsilon_{\text{eff}}\, \hat{E}$$

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

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

An interesting observation about wave transmission

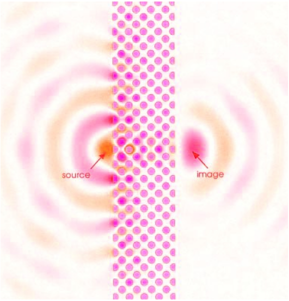


Image taken from

C. Luo, S. G. Johnson, J. D. Joannopoulos, and J. B. Pendry. All-angle negative refraction **without negative effective index.** *Phys. Rev. B, 65:201104, May 2002*

Our motivation:

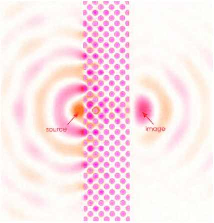
Is this negative refraction at a photonic crystal?

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

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

These two facts can explain negative refraction

This talk



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

- Homogenious media (Sommerfeld, 1912)
- Periodic media (Fliss and Joly, 2016)
- Periodic media with an interface (Lamacz and S., 2016)

Radiation for homogeneous media: Sommerfeld, 1912

Homogeneous problem $-\Delta u = \omega^2 u$ in $\mathbb{R}^n$

Fundamental solutions

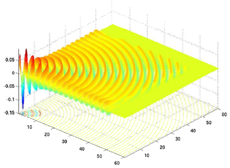
Two fundamental Helmholtz solutions for $x \in \mathbb{R}^3$:

$$u_+(x) := \frac{1}{|x|} e^{i\omega|x|} \quad \text{and} \quad u_-(x) := \frac{1}{|x|} e^{-i\omega|x|}$$

Time-dependence $e^{-i\omega t}$ implies: u_+ is an outgoing wave, u_- an incoming wave.

Sommerfeld condition

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

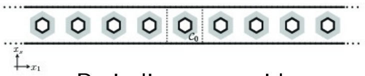


Both elementary solutions decay for $|x| \to \infty$. It is not reasonable to demand only a decay property

- u_+ satisfies (1), it is admissible
- u_- does not satisfy (1), it is not admissible

Justification (Sommerfeld): Radiation condition implies uniqueness

Radiation in a periodic wave-guide: Fliss and Joly, 2016



Periodic wave-guide
$-\nabla \cdot (a\nabla u) = \omega^2 u$

Image taken from *S. Fliss and P. Joly. Solutions of the time-harmonic wave equation in periodic waveguides: asymptotic behaviour and radiation condition. Arch. Ration. Mech. Anal., 219, 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)

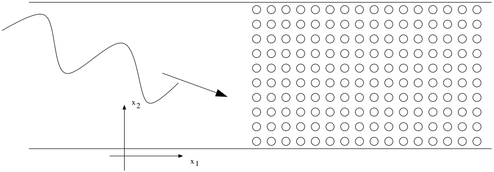
A function u solves the outgoing radiation condition to the right if

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

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

Justification: Radiation condition implies existence and uniqueness

Radiation in media with an interface



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.) $f : \mathbb{R}^n \to \mathbb{R}$ 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.) ξ is written as $\xi = k + j$ with $k \in \mathbb{Z}^n$ and $j \in [0,1)^n =: Z$

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

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

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

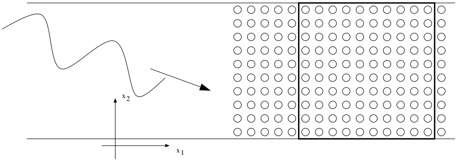
$U_{j,m}(x) := \Psi_{j,m}(x) e^{2\pi i j \cdot x}$ solves

$$-\nabla \cdot (a(x) \nabla U_{j,m}(x)) = \mu_{j,m} U_{j,m}(x)$$

Result: The operator $L = -\nabla \cdot (a(.)\nabla)$ acts as a multiplier:

$$f(x) = \int_Z \sum_{m \in \mathbb{N}} \alpha_{j,m} U_{j,m}(x) \, dj, \qquad Lf = \int_Z \sum_{m \in \mathbb{N}} \alpha_{j,m} \mu_{j,m} U_{j,m}(x) \, dj$$

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

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

Expansion of an arbitrary function u in Bloch waves

Idea: For **"outgoing solutions"** we demand:

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

Note: u periodic $\longrightarrow$ Bloch expansion is a sum

Energy transport of Bloch waves

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_λ^+ describes the right-going energy:

$$P_\lambda^+ := \operatorname{Im} \int_{Y_\varepsilon} \bar{U}_\lambda^+(x)\, e_1 \cdot \left[a^\varepsilon(x) \nabla U_\lambda^+(x)\right]\, dx$$

Index sets: Left-going waves and "vertical waves"

$$I_{<0}^+ := \left\{\lambda \in I \mid P_\lambda^+ < 0\right\} \quad \text{and} \quad I_{=0}^+ := \left\{\lambda \in I \mid P_\lambda^+ = 0\right\}$$

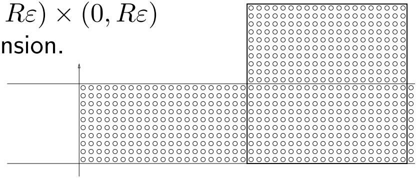
Projection: Onto left-going waves

$$\Pi_{<0}^+ u(x) := \sum_{\lambda \in I_K \cap I_{<0}^+} \alpha_\lambda^+ U_\lambda^+(x)$$

Outgoing wave condition

Given: $u \in L^2_{\mathrm{loc}}(\mathbb{R} \times (0,h); \mathbb{C})$. Height $h = \varepsilon K$.
Large factor $R \in K\mathbb{N}$, $RY_\varepsilon = (0, R\varepsilon) \times (0, R\varepsilon)$
$\tilde{u} : \mathbb{R}^2 \to \mathbb{C}$ 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)

$$\fint_{RY_\varepsilon} \left|\Pi^+_{<0}(u_R^+)\right|^2 \to 0 \text{ as } R \to \infty$$

Our wish-list

Transmission problem

a constant on the left, periodic on the right

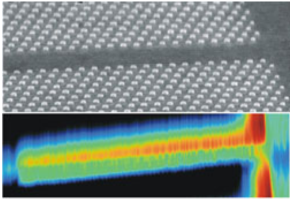
Helmholtz equation: $-\nabla \cdot (a\nabla u) = \omega^2 u$, periodic in vertical direction

Outgoing wave conditions, on the right:

$$\int_{RY_\varepsilon} \left|\Pi^+_{<0}(u^+_R)\right|^2 \to 0 \text{ as } R \to \infty$$

Wishful thinking: For *every* frequency $\omega > 0$

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



S. Bozhevolnyi/Aalborg Univ.

Uniqueness cannot be expected

There are surface-waves $\longrightarrow$ no uniqueness!

Bloch measures

G. Allaire and C. Conca. Bloch wave homogenization and spectral asymptotic analysis. J. Math. Pures Appl. 1998

Let $u_R \in L^2(W_R; \mathbb{C})$ be a sequence

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

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

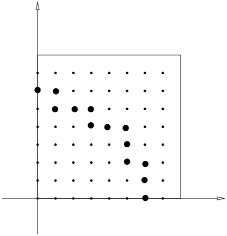
$$\nu_{l,R}^\pm := \sum_{\lambda=(j,l) \in I_R} |\alpha_\lambda^\pm|^2 \ \delta_j$$

where δ_j denotes the Dirac measure in $j \in Z$.
If, as $R \to \infty$,

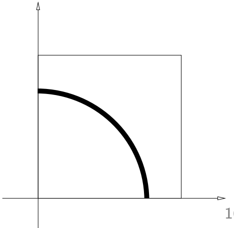
$$\nu_{l,R}^\pm \to \nu_{l,\infty}^\pm$$

in the sense of measures, then

$\nu_{l,\infty}^\pm \in \mathcal{M}(Z)$ is a Bloch measure generated by u



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



Uniqueness result

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

$$\omega^2 < \inf_{j \in Z,\, m \geq 1} \mu_m^{+}(j) \qquad (3)$$

Theorem (Uniqueness)

Let two solutions u and $\tilde{u}$ of the transmission problem. Then the difference $v := u - \tilde{u}$ generates a Bloch measure that has support only on vertical waves.

Corollary for *non-singular frequencies ω:* The Bloch measure of the difference v vanishes.

Interpretation: Waves can be

- localized at the interface
  or
- travelling vertically in the photonic crystal

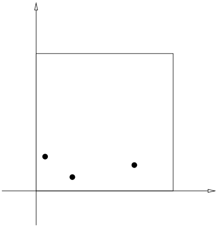


Figure: The indices $j \in Z$ corresponding to "vertical waves"

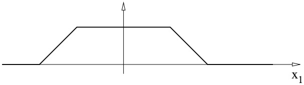
Uniqueness follows from energy conservation

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

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

Let v solve the Helmholtz equation with coefficients $a = a^{\varepsilon}$, use

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



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

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

Take the imaginary parts and obtain the energy conservation

$$\operatorname{Im} b_R^{-}\left(v_R^{-}, v_R^{-}\right) = \operatorname{Im} b_R^{+}\left(v_R^{+}, v_R^{+}\right)$$

Result: If both terms have opposite sign, they must vanish!

Show $\nu^{\pm}_{l,\infty} = 0$ for $l \geq 1$

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

$$\begin{aligned}
\delta \fint_{W_R} \left|\Pi^{\mathrm{ev},+}_{m\geq 1}(u_R^+)\right|^2 &= \delta \sum_{\substack{\lambda=(j,m)\in I_R \\ m\geq 1}} \left|\left\langle u_R^+ , U_\lambda \right\rangle_R\right|^2 \\
&\leq \sum_{\substack{\lambda=(j,m)\in I_R \\ m\geq 1}} \left|(\omega^2 - \mu_\lambda)\langle u_R^+ , U_\lambda\rangle_R\right|^2 \\
&\leq \sum_{\lambda\in I_R} \left|\left\langle \omega^2 u_R^+ , U_\lambda \right\rangle_R - \left\langle \mu_\lambda u_R^+ , U_\lambda \right\rangle_R\right|^2 \\
&= \sum_{\lambda\in I_R} \left|\left\langle \mathcal{L}_0(u_R^+) , U_\lambda \right\rangle_R - \left\langle \mu_\lambda u_R^+ , U_\lambda \right\rangle_R\right|^2 = 0
\end{aligned}$$

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

A similar calculation yields: $\quad \mathrm{supp}(\nu^{\pm}_{0,\infty}) \subset \left\{ j \in Z \,|\, \mu^{\pm}_0(j) = \omega^2 \right\}$

Transmission condition

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

Theorem (Transmission conditions)

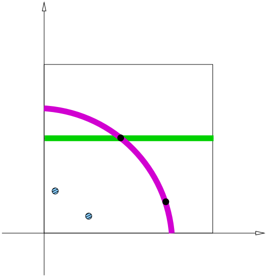
Let u be a solution of the transmission problem.
Let $\nu^{\pm}_{l,\infty}$ be a Bloch measure to u.

Then: $\nu^{\pm}_{l,\infty} = 0$ *for* $l \geq 1$,

$$\mathrm{supp}(\nu^{\pm}_{0,\infty}) \;\subset\; \{j \in Z \,|\, \mu^{\pm}_0(j) = \omega^2\}$$

and

$$\mathrm{supp}(\nu^{\pm}_{0,\infty}) \;\subset\; \{j \in Z \,|\, j_2 = k_2\} \;\cup\; J^{\pm}_{=0,0}$$



Waves must have:

- the correct energy **and**
- the correct k_2 (or be vertical)

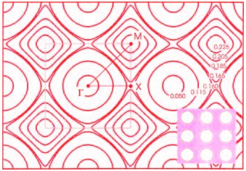
The theorem follows from uniqueness: Compare u with its projection to the vertical wave number k_2

Conclusions and open problems

Corollary for *non-singular frequencies ω:*

The Bloch measure of u is supported on $\{j \in Z \,|\, j_2 = k_2\}$.

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?

Thank you!