Waves in unbounded photonic crystals and transmission properties at interfaces

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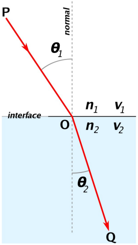
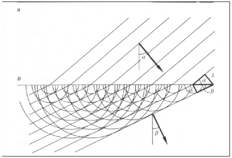
Geometric optics vs. Wave equation

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

Light finds the fastest way to reach the destination!

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

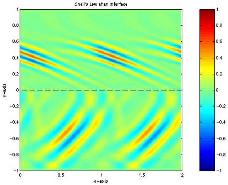




Huygens' principle of **superpositions**

Wave equation

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



Numerical solution

Maxwell's equations and negatve index

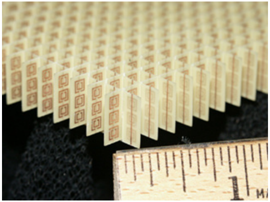
Maxwell's Equations (1865)

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

E: electric field, H: magnetic field

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

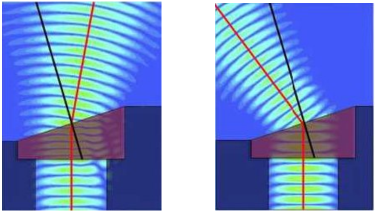
- $\operatorname{Re}\varepsilon < 0$ possible
- μ is always 1
- $\operatorname{Re}\mu\varepsilon < 0$: medium is opaque



Veselago (1968)

Materials with negative index

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

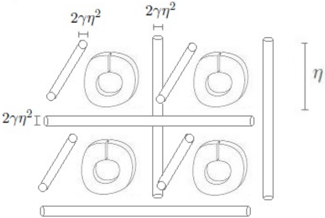


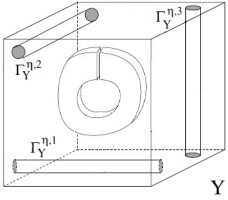
Solutions for positive and negative index

Pendry et al. ($\sim$ 2000)

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

Microscopic 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., SIAM J.Math.Anal. 2017)

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

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

$$\mu_{\mathsf{eff}} = \mu_{\mathsf{eff,R}} \quad \text{and} \quad \varepsilon_{\mathsf{eff}} = \varepsilon_{\mathsf{eff,R}} + \pi\gamma^2\, \varepsilon_W\,.$$

Wave transmission into photonic crystals

Our motivation:

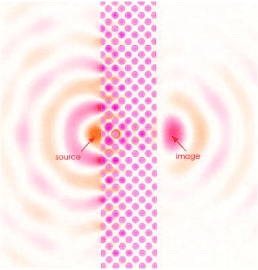
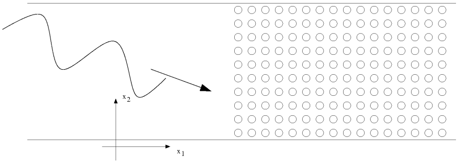


Image taken from

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*

Is this negative refraction at a photonic crystal?



Geometry of the transmission problem.

We study the waves that are generated in the photonic crystal.

Helmholtz equation:

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

Bloch expansion: Write an arbitrary function f in a smart way!

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

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

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

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

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

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

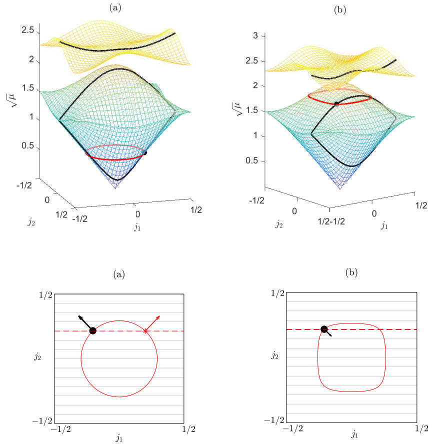
$U_{j,m}(x) := \Psi_{j,m}(x) e^{2\pi \mathrm{i} j \cdot x}$ solves

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

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

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

Energy landscape in the periodic medium



The three surfaces correspond to $m = 0, 1, 2$.
The vertical axis shows $\sqrt{\mu_{j,m}}$, where $\mu_{j,m}$ is the m-th eigenvalue for the wave vector $j = (j_1, j_2)$.

The arrows show gradients of the energy landscape

Energy transport by Bloch waves

For $\lambda = (j, m)$, which Bloch wave U_λ is "right going"?

Recall for Maxwell: The Poynting vector $P := E \times H$ measures the energy flux

Poynting number

The Poynting number P_λ describes the right-going energy:

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

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

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

Radiation for homogeneous media: Sommerfeld, 1912

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

Fundamental solutions

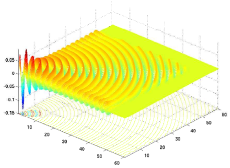
Two fundamental Helmholtz solutions for $x \in \mathbb{R}^3$:

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

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

Sommerfeld condition

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

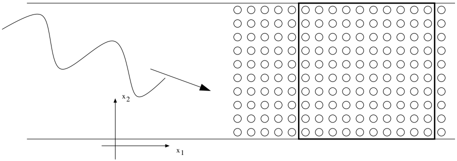


Both elementary solutions decay for $|x| \to \infty$. It is not reasonable to demand only a decay property

- u_+ satisfies the Sommerfeld condition
- u_- does not

Justification (Sommerfeld): Radiation condition implies uniqueness

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

For “outgoing solutions” we demand (on the right):

u consists only of right-going Bloch modes

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

Our wish-list

Transmission problem

a constant on the left, periodic on the right

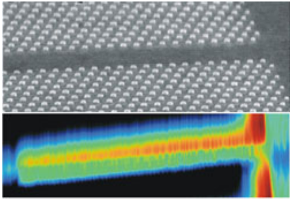
Helmholtz equation: $-\nabla \cdot (a\nabla u) = \omega^2 u$, periodic in vertical direction

Outgoing wave conditions, on the right:

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

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 $l \in \mathbb{N}_0$:

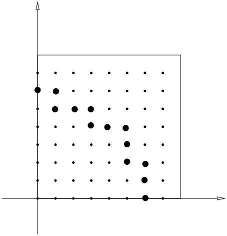
$$\nu_{l,R}^\pm := \sum_{\lambda=(j,l)\in I_R} |\alpha_\lambda^\pm|^2 \;\; \delta_j$$

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

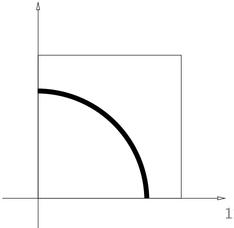
$\nu_{l,\infty}^\pm \in \mathcal{M}(Z)$ is a Bloch measure generated by u



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 $\mu_m^{\pm}(j)$:

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

Theorem (A.Lamacz & B.S., Uniqueness)

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

Interpretation: Waves can be

- localized at the interface

  or

- travelling vertically in the photonic crystal

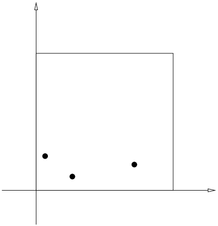
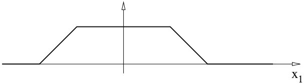


Figure: The indices $j \in Z$ corresponding to "vertical waves"

Uniqueness follows from energy conservation

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 $\vartheta(x)\,\overline{v}(x)$ to obtain

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

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

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

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 $\nu_{l,\infty}^{\pm} = 0$ 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,

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

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

A similar calculation yields: $\quad \mathrm{supp}(\nu_{0,\infty}^{\pm}) \subset \left\{ j \in Z \,|\, \mu_0^{\pm}(j) = \omega^2 \right\}$

Transmission conditions

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

Theorem (Transmission conditions)

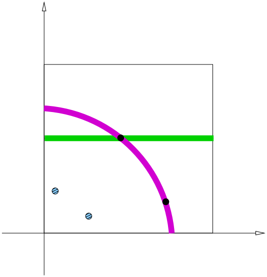
Let u be a solution of the transmission problem.
Let $\nu^{\pm}_{l,\infty}$ be a Bloch measure to u.

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

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

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)

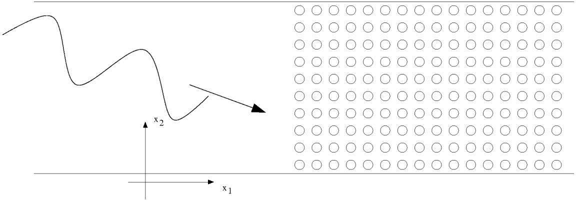
The theorem follows from uniqueness: Compare u with its projection to the vertical wave number k_2

A numerical scheme

Based on the radiation condition $\longrightarrow$ numerical scheme

T. Dohnal and B. Schweizer: A Bloch wave numerical scheme for scattering problems in periodic wave-guides (submitted)

$$-\nabla \cdot (a\nabla u) = \omega^2(1 + \mathrm{i}\delta)u + f$$



Concept:

- At the far left/right:
  Solution is a linear combination of outgoing Bloch waves
- Standard finite elements in the core domain

Design of the scheme, negative refraction

In the radiation boxes $W_{R,L}^{\pm}$ use $X^{\pm} := span\{U_{\lambda}^{\pm} \mid \lambda \in I^{\pm}\}$,
The index sets $I^{\pm}$ satisfy $\lambda \in I^{\pm} \Rightarrow \pm P_{\lambda}^{\pm} > 0$.

Function space:

$$V := \left\{ u \in H^1(\Omega_{R+L}) \,\middle|\, u \text{ vertically periodic, } \{u\}_{R,L}^{+} \in X^{+}, \{u\}_{R,L}^{-} \in X^{-} \right\}$$

Bilinear form (with cut-off function ϑ as above):

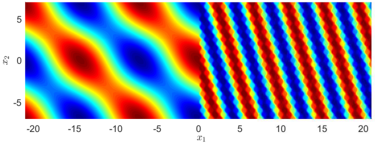
$$\beta(u,v) := \int_{\Omega_{R+L}} a\nabla\bar{u}\cdot\nabla v\,\vartheta - \int_{\Omega_{R+L}} (1 - \mathrm{i}\delta\mathbf{1}_{\Omega_R})\,\omega^2\bar{u}\,v\,\vartheta$$
$$- \frac{1}{\varepsilon L}\int_{W_{R,L}^{+}} a\nabla\bar{u}\cdot e_1\,v + \frac{1}{\varepsilon L}\int_{W_{R,L}^{-}} a\nabla\bar{u}\cdot e_1\,v = \int_{\Omega_R} \bar{f}\,v$$

Coercivity of β follows from $\nabla\vartheta = \mp\frac{1}{L}e_1$ and $P_{\lambda}^{\pm} > 0$.

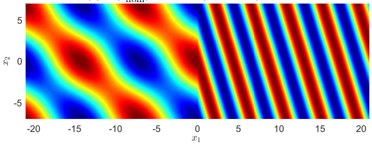
Numerical results: Comparison with homogenization

Transmission into periodic medium I: Large wave-length

(a) $\mathrm{Re}(u)$ for $k^{(\mathrm{in})} \approx (0.440, 0.449), \omega_0 = 0.2\pi$

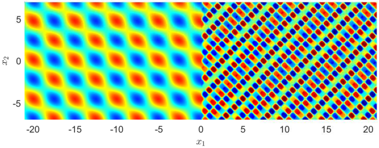


(b) $\mathrm{Re}(u_{\mathrm{hom}})$ for $k^{(\mathrm{in})} \approx (0.440, 0.449), \omega_0 = 0.2\pi$

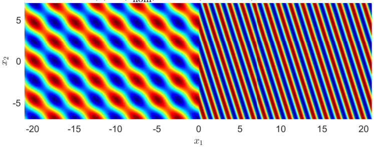


Transmission II: Wave-length comparable to structure

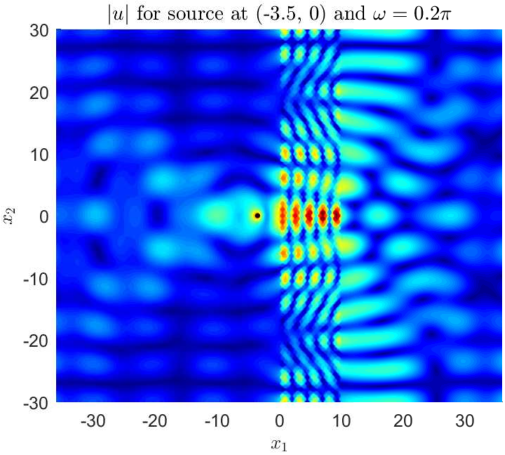
(a) $\mathrm{Re}(u)$ for $k^{(\mathrm{in})} \approx (1.269, 1.346), \omega_0 = 1.85$



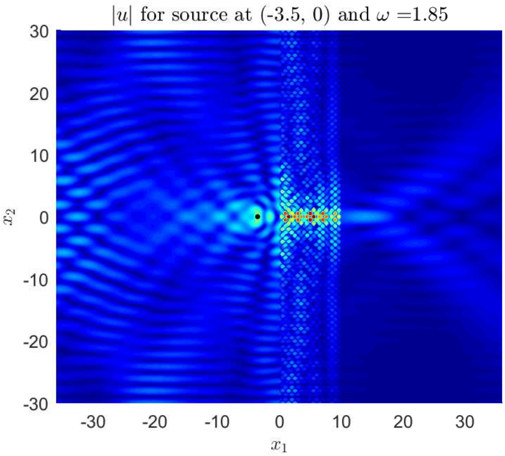
(b) $\mathrm{Re}(u_{\mathrm{hom}})$: $k^{(\mathrm{in})} \approx (1.269, 1.346)$, $\omega_0 = 1.85$



A finite crystal with positive refraction property



A finite crystal with negative refraction property



Thank you!