Some unconventional PDE problems from photonics

Robert V. Kohn Courant Institute, NYU

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Robert V. Kohn Unconventional PDE problems from photonics

Talk plan

Photonics can lead to PDE problems rather different from the ones we usually study.

I'll discuss a couple of examples (very briefly), then tell you a story about one such problem.

(1) Introduction: some examples

- negative-epsilon inclusions with corners
- ENZ-based waveguides

(2) Today's story: geometry-invariant resonant cavities

- Formulation as a PDE problem
- Existence and robustness of resonances
- An associated optimal design problem
- Work with Raghav Venkatraman (now at Univ of Utah), inspired by discussions with Nader Engheta (Penn).

Electromagnetic waves are described by Maxwell's equations. In the time-harmonic TM setting, where $H = (0, 0, u(x_1, x_2))$ and $E = \frac{1}{l\omega\varepsilon}(-\partial_2 u, \partial_1 u, 0)$, Maxwell reduces to a 2D scalar eqn

$$\nabla \cdot \left(\frac{1}{\varepsilon(x,\omega)}\nabla u\right) + \omega^2 \mu(x,\omega)u = 0$$

where $\omega =$ frequency, and $\varepsilon(x, \omega), \mu(x, \omega)$ are the permittivity and permeability (describing the response of the material at *x*).

This is not a linear eigenvalue problem when ε and μ depend on ω . What if ε is negative? Then the operator loses ellipticity.

What if ε is nearly 0 in some region? Then the operator is singular, but the expected behavior is very simple: *u* should be nearly constant in such a region. My main story will have this character.

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Negative-epsilon inclusions

Let's focus on the principal part, which has the form: $\nabla \cdot (a(x)\nabla u)$ with $a(x) = 1/\varepsilon(x)$. If $\varepsilon(x)$ changes sign, it isn't elliptic.

A basic question: can we solve bvp's for negative-epsilon inclusions? Up to normalization, this concerns

$$abla \cdot (a(x)\nabla u) = 0 \quad \text{in } \Omega$$

 $u = u_0 \quad \text{at } \partial \Omega$



where

 $a(x) = \left\{ egin{array}{cc} -lpha & ext{in inclusion } (lpha > 0 ext{ real}) \ 1 & ext{outside} \end{array}
ight.$

For C^1 inclusions, a boundary integral method works except when $\alpha = 1$. It inverts an operator of the form $c(\alpha)I + K$ with $c(\alpha) = \frac{1-\alpha}{1+\alpha}$ and K compact. Fredholm alternative applies.

The case $\alpha = 1$ is very different. It is the regime of anomalous localized resonance, see e.g. Nguyen, SIAM J Math Anal 2017.

Negative-epsilon inclusions

$$\nabla \cdot (a(x)\nabla u) = 0 \quad \text{in } \Omega$$

$$u = u_0 \quad \text{at } \partial \Omega$$

$$a(x) = \begin{cases} -\alpha & \text{in inclusion } (\alpha > 0 \text{ real}) \\ 1 & \text{outside} \end{cases}$$

For inclusions with corners, the situation is very different.

Fundamental reason: to guess behavior near corner, look for solution of form $r^{\xi}\phi(\theta)$. One finds that ξ is purely imaginary when corner angle β satisfies when $\frac{\beta}{2\pi-\beta} < \alpha < \frac{2\pi-\beta}{\beta}$.

Problem is ill-posed (since changing *i* to -i gives two solutions).

Ill-posedness is resolved by including loss (i.e. giving ε a nonzero imaginary part).

Representative refs: Bonnet-Ben Dhia et al, J Comp Phys 2021; Bonnetier & Zhang, Revista Matematica Iberoamericana 2019.

Waveguide design using ENZ materials



A flat waveguide is studied using sep of var: when ε is a piecewise-constant function of x_1 , soln in each part is lin combn of $\phi_j(x_2)e^{ik_jx_1}$ where ϕ_j is an eigenfn of $-\partial_2^2\phi_j = \lambda_j\phi$ and $\omega^2\varepsilon\mu - k_j^2 = \lambda_j$.

But if $\varepsilon \approx 0$ in a segment then $\nabla u \approx 0$ there. In this region we aren't really solving a PDE; rather, we are choosing a constant. So this region shouldn't have to be flat.

Reflection vs transmission depends on value of μ and area of ENZ region. However, we can get more control by introducing a non-ENZ inclusion in the ENZ region ("photonic doping").

Some refs: Silveirinha & Engheta, PRL 2006 and Phys Rev B 2007; Liberal et al, Science 2017; Kohn & Venkatraman, CPAM 2023.

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Why can permittivity be zero or negative?

The electric field $\mathcal{E}(x, t)$ and magnetic field $\mathcal{H}(x, t)$ satisfy

$$\nabla \times \mathcal{E} = -\partial_t \mathcal{B}, \quad \nabla \times \mathcal{H} = \partial_t \mathcal{D}$$

where $\mathcal D$ (electric displacement) and $\mathcal B$ (magnetic induction) are divergence-free.

In free space, $\mathcal{D} = \varepsilon_0 \mathcal{E}$ and $\mathcal{B} = \mu_0 \mathcal{H}$. However, in materials the constitutive relations are nonlocal in time:

$$\mathcal{D}(x,t) = \int_{-\infty}^{t} f(x,t-t')\mathcal{E}(x,t') dt' \quad \mathcal{B}(x,t) = \int_{-\infty}^{t} g(x,t-t')\mathcal{H}(x,t') dt'$$

Light excites the electrons; it takes a while for them to settle down.

The fields *E* and *H* in time-harmonic Maxwell system are Fourier transforms of \mathcal{E} and \mathcal{H} . Since FT turns convolution into multiplication, the constitutive relation becomes local:

$$D(x,\omega) = \varepsilon(x,\omega)E(x,\omega) \quad B(x,\omega) = \mu(x,\omega)H(x,\omega)$$

Why can permittivity be zero or negative?

Informally: light excites the electrons, and it takes a while for them to settle down.

Precisely: as freq ω varies over positive reals, $\varepsilon(\omega)$ has (damped) resonances. Near a resonance, it can be fit to a Lorentz model:



 $\gamma > 0$ represents loss; $\gamma = 0 \Rightarrow$ singular at $\omega = \omega_0$ solid blue curve is $Re(\varepsilon)$; dotted green curve is $Im(\varepsilon)$ Near a resonance, $Re(\varepsilon)$ can take virtually any value; moreover, $Im(\varepsilon)$ can be small near ENZ freq.

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R.V. Kohn and R. Venkatraman, *Transverse magnetic ENZ resonators: Robustness and optimal shape design*, Arch. Rational Mech. Anal. 248, 2024 (also available as arXiv:2403.11242).

Geometry-invariant resonant cavities

Liberal, Mahmoud, Engheta, Nature Comm 2016

Can one design a resonator by placing a non-ENZ inclusion in an ENZ shell, isolated by a perfectly conducting boundary?



Roughly speaking, this means finding Ω , D, ω , and u such that

$$\nabla \cdot \left(\frac{1}{\varepsilon(x)}\nabla u\right) + \omega^2 \mu u = 0$$

(with $\partial_{\nu} u = 0$ at $\partial \Omega$), when $\varepsilon(x) = 0$ in ENZ region.

- In ENZ limit, only area of ENZ shell will matter (not shape) for existence of desired resonance.
- PDE on left is sloppy. Actually, the dielectric permittivity of a material depends on frequency: ε = ε(ω).
- Moreover, materials have losses; therefore ε should be a small complex number in the ENZ region. The resonant frequency is then also complex, with neg imag part (so $e^{-i\omega t}u(x)$ decays as $t \to \infty$).

The ENZ limit is an idealization. How robust are its predictions?

Liberal et al understood conditions for existence of a resonance in ENZ limit, but relied on simulations to assess impact of loss.

We use perturbation theory and implicit function theorem to achieve a different type of understanding.

• Sensitivity of resonance to loss is geometry-dependent. How can shape of ENZ shell be chosen to minimize it?

Simulations showed this shape dependence.

We also analyze the optimal design problem.



The PDE problem

Following Liberal et al, we take $\mu = \mu_0$, and we ignore loss in *D*:

$$\varepsilon(\mathbf{x}) = \begin{cases} \varepsilon_0 \varepsilon_D(\omega) & \text{in } D\\ \varepsilon_0 \varepsilon_{\text{ENZ}}(\omega; \gamma) & \text{in } \Omega \setminus D \end{cases}$$



where $\varepsilon_D(\omega)$ is real when ω is real, and ε_{ENZ} is a Lorentz model. We want to solve

$$\nabla \cdot \left(\frac{1}{\varepsilon_D(\omega)} \nabla u\right) + \omega^2 c^{-2} u = 0 \qquad \text{in } D,$$

$$\nabla \cdot \left(\frac{1}{\varepsilon_{\text{ENZ}}(\omega; \gamma)} \nabla u\right) + \omega^2 c^{-2} u = 0 \qquad \text{in } \Omega \setminus D$$

with *u* and $\frac{1}{\varepsilon}\partial u/\partial \nu$ continuous at ∂D , and $\partial u/\partial \nu = 0$ at $\partial \Omega$. (Here $c = 1/\sqrt{\varepsilon_0 \mu_0}$ is the speed of light in vacuum.)

Not a linear eigenvalue problem!

Strategy for analysis

(1) Ignore dispersion and loss. Multiplying eqns by ε_D , PDE becomes

$$\nabla \cdot \left(\varepsilon_{\delta}^{-1} \nabla u_{\delta}\right) + \lambda_{\delta} u_{\delta} = 0$$

with

$$\varepsilon_{\delta} = \begin{cases} 1 & \text{in } D & \delta = \varepsilon_{\text{ENZ}}/\varepsilon_{D} \\ \delta & \text{in } \Omega \setminus D & \lambda_{\delta} = \omega^{2} c^{-2} \varepsilon_{D} \end{cases}$$

We show that u_{δ} and λ_{δ} are analytic functions of δ near $\delta = 0$.

(2) Allow for dispersion and loss using implicit function theorem: find $\omega(\gamma)$ for γ near zero, with $\omega(0) =$ lossless ENZ frequency, so that

$$\lambda_{\varepsilon_{\rm ENZ}(\omega(\gamma);\gamma)/\varepsilon_{\rm D}(\omega(\gamma))} = \omega^2(\gamma) \mathbf{c}^{-2} \varepsilon_{\rm D}(\omega(\gamma))$$

Understanding u_{δ} and λ_{δ}

Obvious starting point – expand in powers of δ :

$$u_{\delta} = \begin{cases} 1 + \delta\phi_1 + \delta^2\phi_2 + \cdots & \text{in ENZ} \\ \psi_* + \delta\psi_1 + \delta^2\psi_2 + \cdots & \text{in } D \end{cases}$$
$$\lambda_{\delta} = \lambda_* + \delta\lambda_1 + \delta^2\lambda_2 + \cdots$$



Leading-order PDE in D:

$$\Delta \psi_* + \lambda_* \psi_* = 0$$
 in *D*, with $\psi_* = 1$ at ∂D .

(Note that ψ_* depends nonlinearly on λ_*).

Leading-order PDE in ENZ region:

$$\begin{split} -\Delta \phi_1 &= \lambda_* \quad \text{in ENZ region} \\ \partial_\nu \phi_1 &= 0 \quad \text{at outer bdry} \\ \partial_\nu \phi_1 &= \partial_\nu \psi_* \quad \text{at } \partial D. \end{split}$$

Consistency fixes (only) ENZ area, if λ_* and *D* are held fixed.

Understanding u_{δ} and λ_{δ}

More detail on the consistency condition: since

$$\begin{split} -\Delta \phi_1 &= \lambda_* \quad \text{in ENZ region} \\ \partial_{\nu} \phi_1 &= 0 \quad \text{at outer bdry} \\ \partial_{\nu} \phi_1 &= \partial_{\nu} \psi_* \quad \text{at } \partial D \end{split}$$



we need

$$-\int_{\partial D} \partial_{\nu} \psi_* = \lambda_*$$
 (Area of ENZ region).

Note that shape of ENZ region doesn't matter – only its area matters.

If ENZ material is fixed, then lossless ENZ frequency ω_* is fixed. So $\lambda_* = \omega_*^2 c^{-2} \varepsilon_D(\omega_*)$ is fixed. The function ψ_* is then determined by D alone. An acceptable ENZ area exists iff $\int_{\partial D} \partial_{\nu} \psi_* < 0$.

For any shape of *D*, this can be assured by suitably scaling the size.

As usual in perturbation of eigenvalue problems, correction to eigenvalue is given in terms of correction to eigenfunction:

$$u_{\delta} = \begin{cases} 1 + \delta\phi_{1} + \delta^{2}\phi_{2} + \cdots & \text{in ENZ} \\ \psi_{*} + \delta\psi_{1} + \delta^{2}\psi_{2} + \cdots & \text{in } D \end{cases} \qquad \lambda_{1} = \frac{-\int_{\text{ENZ}} |\nabla\phi_{1}|^{2}}{A_{\text{ENZ}} + \int_{D} \psi_{*}^{2}}$$

where A_{ENZ} is area of ENZ region. So λ_1 is a negative real number, and it DOES depend on shape of ENZ region.

When we introduce loss, leading-order effect is proportional to λ_1 . Hence the optimal design problem: what shape ENZ region minimizes $|\lambda_1|$? Leading-order terms were found by (i) solving a Helmholtz eqn in D for ψ_* , then (ii) solving a Poisson-type PDE in ENZ region for ϕ_1 . With good organization, entire expansion can be found similarly.

But there's a more elegant way: knowing the leading-order corrections lets us desingularize the problem:

$$u_{\delta} = \begin{cases} 1 + \delta\phi_{1} + \delta^{2}\phi_{2} + \cdots &= 1 + \delta f_{\delta} & \text{in ENZ} \\ \psi_{*} + \delta\psi_{1} + \delta^{2}\psi_{2} + \cdots &= \psi_{*} + \delta g_{\delta} & \text{in } D \\ \lambda_{\delta} = \lambda_{*} + \delta\lambda_{1} + \delta^{2}\lambda_{2} + \cdots &= \lambda_{*} + \delta\mu_{\delta} \end{cases}$$

Substitution into

$$abla \cdot \left(arepsilon_{\delta}^{-1}
abla u_{\delta}
ight) + \lambda_{\delta} u_{\delta} = \mathbf{0}$$

gives nonsingular PDE's and bdry conds for f_{δ} , g_{δ} , and μ_{δ} .

We apply implicit function theorem to get existence and analyticity of solutions with $f_0 = \phi_1$, $g_0 = \psi_1$, and $\mu_0 = \lambda_1$.

Recall: fixing *D*, λ_* , and A_{ENZ} (since these are coupled), optimal design problem seeks shape of ENZ region that minimizes $|\lambda_1|$ (where $\lambda_{\delta} = \lambda_* + \delta \lambda_1 + \cdots$).

This is a compliance optimization problem, since

$$\lambda_1 = -c \int_{\mathrm{ENZ}} |
abla \phi_1|^2$$

$$-\Delta \phi_1 = \lambda_* \quad \text{in ENZ region}$$

$$\partial_{\nu} \phi_1 = 0 \quad \text{at outer bdry}$$

$$\partial_{\mu} \phi_1 = \partial_{\mu} \psi_* \quad \text{at } \partial D.$$

where c is a positive constant.

Some such problems have only "homogenized" solutions. In this setting, that would mean ENZ region might have many "holes" (each with a homogeneous Neumann bc).

Compliance problems are well-understood (i) when mixing 2 materials (rather than a region with holes), and (ii) even for holes, if design doesn't affect "source terms" of PDE (alas, not our situation).

Using lessons from the past, we proceed variationally:

$$\max_{\text{ENZ shapes}} - \int_{\text{ENZ}} \int \frac{1}{2} |\nabla \phi_1|^2$$
$$= \max_{\text{ENZ shapes}} \min_{w} \int_{\text{ENZ}} \left[\frac{1}{2} |\nabla w|^2 - \lambda_* w \right] + \int_{\partial D} (\partial_{\nu} \psi_*) w$$



No need to impose area constraint: min over w is $-\infty$ if a candidate ENZ shell has the wrong area.

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No need to impose area constraint: min over w is $-\infty$ if a candidate ENZ shell has the wrong area. Rewriting: our goal is

$$\max_{a(x)=0 \text{ or } 1} \min_{w} \int_{R^{2} \setminus D} a(x) \left[\frac{1}{2} |\nabla w|^{2} - \lambda_{*} w \right] + \int_{\partial D} (\partial_{\nu} \psi_{*}) w$$

$$\leq \max_{0 \leq \theta(x) \leq 1} \min_{w} \int_{R^{2} \setminus D} \theta(x) \left[\frac{1}{2} |\nabla w|^{2} - \lambda_{*} w \right] + \int_{\partial D} (\partial_{\nu} \psi_{*}) w$$

Conjecture: equality holds in last line, since for homogenization limits, $\langle a_{\rm eff} \nabla u, \nabla u \rangle \leq ({\rm arithmetic mean}) |\nabla u|^2.$



Convex duality gives this problem a simple, attractive form:

$$\max_{\substack{0 \le \theta(x) \le 1 \\ w}} \min_{\substack{w}} \int_{R^2 \setminus D} \theta(x) \left[\frac{1}{2} |\nabla w|^2 - \lambda_* w \right] + \int_{\partial D} (\partial_\nu \psi_*) w$$
$$= \min_{\substack{w}} \max_{\substack{0 \le \theta(x) \le 1 \\ 0 \le \theta(x) \le 1}} SAME$$
$$= \min_{\substack{w}} \int_{R^2 \setminus D} \left(\frac{1}{2} |\nabla w|^2 - \lambda_* w \right)_+ + \int_{\partial D} (\partial_\nu \psi_*) w$$

This problem has at least one saddle point: a pair $(\overline{w}, \overline{\theta})$ such that \overline{w} achieves min_w when $\theta = \overline{\theta}$, and $\overline{\theta}$ achieves max_{θ} when $w = \overline{w}$.

When *D* is a ball, optimal ENZ shell is a concentric annulus. Associated \overline{w} and $\overline{\theta}$ are a saddle point of relaxed pbm, so they solve it. Since relaxation wasn't used, they also solve unrelaxed pbm.



Is homogenization ever needed? If so, then $0 < \overline{\theta} < 1$ and $\frac{1}{2} |\nabla \overline{w}|^2 - \lambda_* \overline{w} = 0$ on a set of pos measure.

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Stepping back

- The time-harmonic Maxwell system reduces, in the TM setting, to a scalar PDE of the form ∇ · (ε⁻¹∇u) + ω²µu = 0.
- Frequency dependence of the permittivity ε can lead to PDE problems where 2nd-order term is singular or non-elliptic.
- The associated phenomena are interesting and can be useful.

One application: resonator made by surrounding an ordinary dielectric with an ENZ shell.



- Usually, eigenvalues of a PDE depend upon shape of domain. Here, only area of ENZ region matters in the lossless limit.
- Loss in ENZ material makes the resonance decay. Shape of the ENZ shell affects decay rate.
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