Mathematical Analysis of Some Devices Made Using Epsilon-Near-Zero Materials

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Inspired by discussions with Nader Engheta (Penn)

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Analysis of devices made from ENZ materials

Talk plan:

(1) The big picture

(2) Photonic doping

(3) ENZ-based resonators

The big picture

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

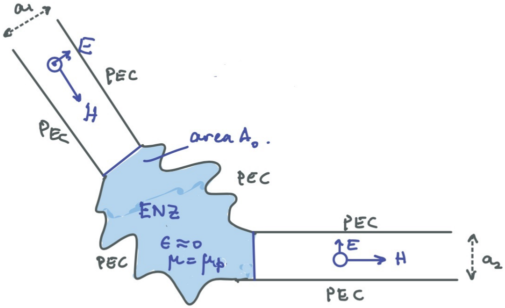
$$\nabla \cdot \left(\frac{1}{\varepsilon(x)} \nabla u \right) + \omega^2 \mu(x) u = \text{sources}$$

where $\omega =$ frequency, and $\varepsilon(x), \mu(x)$ are the permittivity and permeability (typically piecewise constant).

Geometry matters a lot when solving a PDE. But if $\varepsilon(x) = \delta \approx 0$ in some region, then expect $\nabla u \sim \delta$ there. So as $\delta \to 0$, we're not solving a PDE. Thus: geometry of ENZ region shouldn't matter so much.

Application to waveguide design

Silveirinha & Engheta, PRL 2006

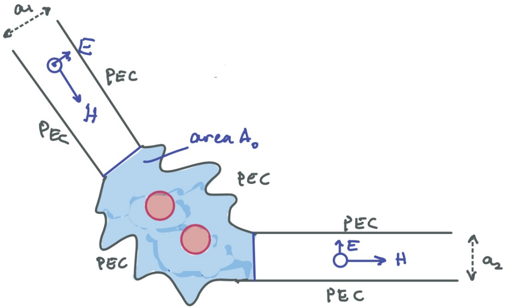


- Parallel plate waveguides joined by ENZ region. (Waveguides meet ENZ region orthogonally.)
- In ENZ limit, reflection coefficient depends on area A_0 of ENZ region but not its shape.
- Faithful transmission ($\rho \approx 0$) when $a_1 \approx a_2$ and A_0 is small.

reflection coefft $\rho = \frac{(a_1 - a_2) + i\omega\mu_\phi A_0}{(a_1 + a_2) - i\omega\mu_\phi A_0}$

Application to waveguide design, cont'd

Silveirinha & Engheta, PRB 2007



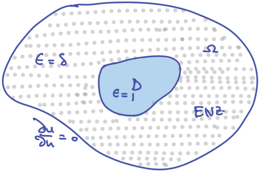
- A follow up paper introduced a new idea: use non-ENZ inclusions to give central region an effective permeability μ_{eff}.
- Then good transmission doesn't require that A_0 be small. It's enough that $\mu_{\text{eff}} A_0 \approx 0$.
- I'll discuss the meaning of μ_{eff} in due course.

reflection coefft $\rho = \frac{(a_1 - a_2) + i\omega\mu_{\text{eff}} A_0}{(a_1 + a_2) - i\omega\mu_{\text{eff}} A_0}$

Application to ENZ-based resonators

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?



This means finding Ω, D, and ω_* such that there's a nonzero solution of

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

when $\varepsilon(x) = 0$ in $\Omega \setminus D$.

- In the ENZ limit, only area of ENZ shell matters (not shape).
- Real materials have losses; to model this, ε should be a small complex number in the ENZ region. The resonant frequency is then also complex.
- The imaginary part of the resonant frequency controls quality of the resonator. It does depend on geometry. What shape optimizes it?

How can mathematics help?

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

Actually $\varepsilon = \varepsilon(\omega) = \varepsilon' + i\varepsilon''$ is a complex-valued function of frequency.

- ε'' may be small, but it's never zero – it corresponds to losses.
- ε' can vanish only at isolated frequencies.

So, the ENZ limit is an idealization. In a real ENZ material, ε is merely small – a complex number δ near 0.

The physics literature has understood the limiting behavior as $\delta \to 0$, but not the leading-order corrections due to

- losses (imaginary part of $\delta > 0$) and
- change of frequency (real part of $\delta \neq 0$).

(It considers these effects through numerics.)

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Asymptotics or calculus?

These are PDE problems with a small parameter δ. Are we doing asymptotics or calculus?

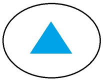
The answer: calculus. Everything is complex-analytic in δ (even for boundaries with corners). Leading-order corrections assoc $\delta \neq 0$ are just the first terms in a Taylor expansion.

As we'll see, leading-order corrections are described by a PDE. (They do feel the geometry of the ENZ region.)

Asymptotics or calculus?

Is it surprising that we're doing calculus, not asymptotics?

Maybe yes: the operator $\nabla \cdot (a(x)\nabla u)$ is not elliptic when $a(x)$ changes sign.



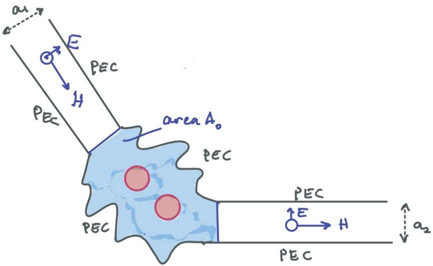
Or maybe not: when $a(x)$ takes just two values, bdry integral version of $\nabla \cdot (a(x)\nabla u) = f$ inverts a Fredholm operator, unless ratio of values is -1.

And yet: bdry integral operators are different for domains with corners; $\nabla \cdot (a(x)\nabla u) = f$ can be ill-posed for other (negative) values of the ratio.

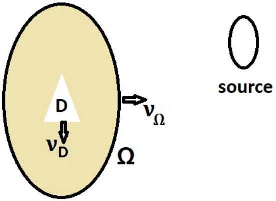
We do not use boundary integrals.

Photonic doping

Recall the second waveguide example, where non-enz inclusions were used to give the central region an effective μ.



I'll capture the essential math by considering a slightly different problem: scattering off a "doped" ENZ obstacle (studied by Liberal et al, Science 2017).



Scattering off a doped ENZ obstacle

For δ complex (near 0), set

$$\varepsilon_\delta(x) = \begin{cases} 1 & x \in D \cup (\mathbb{R}^2 \setminus \overline{\Omega}) \quad \text{(the exterior and dopant)} \\ \delta & x \in \Omega \setminus \overline{D} \quad \text{(the ENZ region)} \end{cases}$$

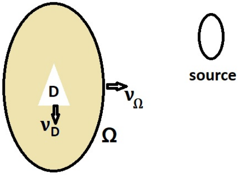
Writing $\omega^2 \mu = k^2$ (and taking k to have nonneg imaginary part), our PDE becomes

$$-\nabla \cdot \frac{1}{\varepsilon_\delta} \nabla u_\delta - k^2 u_\delta = f \quad \text{in } \mathbb{R}^2$$

$$\lim_{r \to \infty} \sqrt{r} \left(\frac{\partial}{\partial r} - ik \right) u_\delta = 0 \quad \text{(radiation condition at } \infty\text{)}$$

Assumptions:

- The source f is supported away from the obstacle.
- The dopant isn't resonant ($k^2 \neq$ Dir eigenval of $-\Delta$ in D).



Getting started

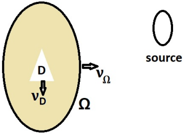
Our strategy: expand solution in powers of δ,

$$u_\delta = v_0 + \delta v_1 + \delta^2 v_2 + \cdots$$

then show the series has a finite radius of convergence.

The first term v_0 term gives the limiting behavior as $\delta \to 0$. It was found in the physics literature:

$$v_0(x) = \begin{cases} c^*\psi_e(x) + s(x) & x \in \text{ exterior} \\ c^* & x \in \text{ ENZ region} \\ c^*\psi_d(x) & x \in \text{ dopant.} \end{cases}$$

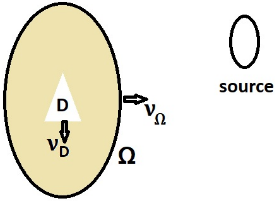


where ψ_e, ψ_d, and s, are certain auxiliary solutions of Helmholtz (to be defined soon), and c^* is a complex constant (to be identified soon).

Auxiliary Problems

$$-\Delta\psi_d = k^2\psi_d \quad \text{in dopant}$$
$$\psi_d = 1 \quad \text{at } \partial D$$

$$-\Delta s = k^2 s + f \quad \text{in exterior}$$
$$s = 0 \quad \text{at } \partial\Omega$$
radiation cond at ∞



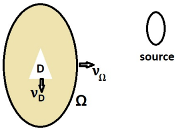
$$-\Delta\psi_e = k^2\psi_e \quad \text{in exterior}$$
$$\psi_e = 1 \quad \text{at } \partial\Omega$$
radiation cond at ∞

The situation thus far

Recall the PDE:

$$-\nabla\cdot(\varepsilon_\delta^{-1}\nabla u_\delta) - k^2 u_\delta = f \quad \text{in } \mathbb{R}^2$$

with the radiation condition at ∞



We expect $u_\delta = v_0 + \delta v_1 + \cdots$. The proposed leading-order term

$$v_0(x) = \begin{cases} c^*\psi_e(x) + s(x) & x \in \text{ exterior} \\ c^* & x \in \text{ ENZ region} \\ c^*\psi_d(x) & x \in \text{ dopant} \end{cases}$$

is continuous at the boundaries, but

- the value of c^* has not yet been determined, and
- the boundary flux $\frac{1}{\varepsilon_\delta}\partial v_0/\partial \nu$ is not continuous.

Both issues will be fixed at the next order.

The next order term

We expect $u_\delta = v_0 + \delta v_1 + O(\delta^2)$.
Introducing some notation:

$$v_1(x) := \begin{cases} \lambda_0(x) & x \in \text{ exterior} \\ e_0 + \phi_0(x) & x \in \text{ ENZ region} \\ \chi_0(x) & x \in \text{ dopant} \end{cases}$$

with the convention that e_0 is constant and $\int_{\mathrm{ENZ}} \phi_0 = 0$.

Focusing first on the ENZ region: ϕ_0 solves

$$-\Delta\phi_0 = k^2 c^* \quad \text{in ENZ region}$$
$$\partial_\nu \phi_0 = c^* \partial_\nu \psi_e + \partial_\nu s \quad \text{at outer bdry of ENZ}$$
$$\partial_\nu \phi_0 = c^* \partial_\nu \psi_d \quad \text{at dopant bdry.}$$

- ϕ_0 solves a Poisson equation, not Helmholtz
- Consistency determines c^*.
- This ϕ_0 makes the bdry fluxes continuous at leading order.
- The value of e_0 is undetermined. (It is set by the consistency condition at the next order.)

The next-order term and beyond

Recall: $u_\delta = v_0 + \delta v_1 + O(\delta^2)$ with

$$v_1(x) = \begin{array}{ccl} \lambda_0(x) & x \in & \text{exterior} \\ e_0 + \phi_0(x) & x \in & \text{ENZ region} \\ \chi_0(x) & x \in & \text{dopant} \end{array}$$

and we just determined ϕ_0. The functions λ_0 and χ_0 solve

$$-\Delta\lambda_0 = k^2\lambda_0 \quad \text{in exterior}$$
$$\lambda_0 = \phi_0 \quad \text{at outer boundary of ENZ}$$
$$\text{radiation cond at } \infty$$

$$-\Delta\chi_0 = k^2\chi_0 \quad \text{in dopant}$$
$$\chi_0 = \phi_0 \quad \text{at dopant bdry}$$

- With these choices, $v_0 + \delta v_1$ is cont's, solves the PDE up to order δ^1, and flux continuity holds at order δ^0.
- The process can be repeated. The next corrector in ENZ region makes flux continuity hold at order δ^1; it provides Dir bc for next-order correctors in the dopant and exterior; etc.
- The PDE's solved at each stage are similar to those we solved to find ϕ_0, λ_0, and χ_0.
- Resulting series for u_δ has finite radius of convergence, by comparison to a suitable geometric series.

Why is this interesting?

The exterior feels the scatterer only through its Dirichlet-to-Neumann map. In the limit $\delta \to 0$, exterior feels only the constant c^*.

The presence of a dopant changes c^*. A more physical viewpoint: it gives the ENZ scatterer an effective permeability μ_{eff} that's different from its physical permeability μ.

Quantitatively: the consistency condition for ϕ_0 gives

$$c^* := -\frac{1}{\beta} \int_{\partial\Omega} \frac{\partial s}{\partial \nu_\Omega} \, d\mathcal{H}^1$$

where

$$\beta = k^2 |\Omega \setminus \overline{D}| + \int_{\partial\Omega} \frac{\partial \psi_e}{\partial \nu_\Omega} \, d\mathcal{H}^1 - \int_{\partial D} \frac{\partial \psi_d}{\partial \nu_D} \, d\mathcal{H}^1.$$

The value of μ_{eff} induced by the dopant is the value of μ that yields the same c^* without any dopant. Since $k^2 = \omega^2 \mu$, this amounts to

$$\omega^2 \mu_{\mathrm{eff}} |\Omega| + \int_{\partial\Omega} \frac{\partial \psi_e}{\partial \nu_\Omega} \, d\mathcal{H}^1 = \omega^2 \mu |\Omega \setminus \overline{D}| + \int_{\partial\Omega} \frac{\partial \psi_e}{\partial \nu_\Omega} \, d\mathcal{H}^1 - \int_{\partial D} \frac{\partial \psi_d}{\partial \nu_D} \, d\mathcal{H}^1.$$

One easily solves for μ_{eff}.

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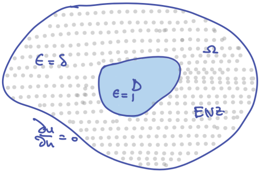
A different application

Design of ENZ-based resonators

Consider resonator made from a non-ENZ inclusion in an ENZ shell, isolated boundary where $\partial u/\partial n = 0$.



This means considering Ω, D, and λ_δ such that there's a nonzero solution of

$$\nabla \cdot \left(\frac{1}{\varepsilon_\delta(x)} \nabla u_\delta \right) + \lambda_\delta u_\delta = 0 \quad \text{in } \Omega$$

with $\partial u_\delta/\partial n = 0$ at $\partial\Omega$; here, as usual,

$$\varepsilon_\delta(x) = \begin{cases} 1 & \text{in } D \\ \delta & \text{in } \Omega \setminus D. \end{cases}$$

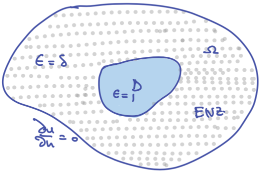
- Both u_δ and λ_δ are analytic functions of δ; moreover $\lambda_\delta = \lambda_* + \delta\lambda_1 + \ldots$ where λ_* and λ_1 are both real.
- To model losses in ENZ region, δ should be taken purely imaginary. This gives λ_δ the leading-order imag part $\delta\lambda_1$.
- Imag part of λ_δ controls decay of the resonance. (In our time-harmonic setting, fields are proportional to $e^{-i\omega t}$ and $\lambda = \omega^2\mu$.)
- This raises the optimal design question: minimize $|\lambda_1|$, to minimize the effect of losses.

Dependence on δ

Proof of analyticity in δ is a lot like the photonic doping example. I'll discuss just the leading-order corrections. One expects

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

$$\lambda_\delta = \lambda_* + \delta\lambda_1 + \delta^2\lambda_2 + \cdots$$



where each ϕ_j has mean 0, and ψ_d solves (as usual) $-\Delta\psi_d = \lambda_*\psi_d$ in D, with $\psi_d = 1$ at ∂D.

Leading-order PDE gives ϕ_1:

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

Consistency restricts λ_*. The possibilities are discrete, but there are infinitely many (and λ_* is never a Dir eigenvalue of $-\Delta$ in D).

The optimal design problem

As usual in perturbation theory of eigenvalues, leading-order correction of the eigenvalue is related to leading-order correction of eigenfunction. In fact: $\lambda_\delta = \lambda_* + \delta\lambda_1 + \dots$ with

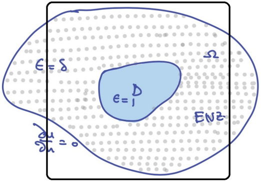
$$\lambda_1 = \frac{-\int_{\mathrm{ENZ}} |\nabla \phi_1|^2}{A_{\mathrm{ENZ}} + \int_D \psi_d^2}$$

where A_{ENZ} is the area of the ENZ region $\Omega \setminus D$.

Our optimal design problem is to minimize $|\lambda_1|$. The conditions that determine λ_* and the denominator of the expression for λ_1 depend only on the area of he ENZ region. So our optimal design problem amounts to

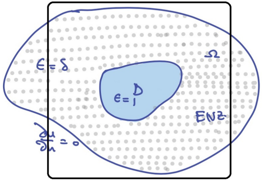
$$\max_{A_{\mathrm{ENZ}}=\mathrm{const}} - \int_{\mathrm{ENZ}} \int \tfrac{1}{2}|\nabla \phi_1|^2$$

$$= \max_{A_{\mathrm{ENZ}}=\mathrm{const}} \min_w \int_{ENZ} \tfrac{1}{2}|\nabla w|^2 - \lambda_* w - \int_{\partial D} (\partial_\nu \psi_d) w$$



A result on the optimal design problem

$$\max_{A_{\mathrm{ENZ}}=\mathrm{const}} - \int_{\mathrm{ENZ}} \int \frac{1}{2} |\nabla \phi_1|^2$$
$$= \max_{A_{\mathrm{ENZ}}=\mathrm{const}} \min_{w} \int_{ENZ} \tfrac{1}{2} |\nabla w|^2 - \lambda_* w - \int_{\partial D} (\partial_\nu \psi_d) w$$



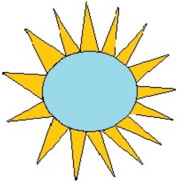
When D is a circle, the optimal ENZ shell is a concentric annulus.

Sketch of the proof:

- When D is a circle and the ENZ shell is an annulus, $\phi_1 = \phi_1(r)$ is very explicit. It is an increasing function of r. Since the value at the outer boundary is constant, we can extend it (using this constant value) to all $\mathbb{R}^2$.
- Use this extension of ϕ_1 as a test function w in the variational characterization of λ_1.

Work in progress on the optimal design problem

In general, we believe one must look for a "relaxed" solution. This leads (at least formally) to a convex optimization.



If $\theta(x)$ is the local volume fraction of the ENZ region, the relaxed problem is

$$\max_{\int \theta(x)=\text{const}} \min_{w} \int_{\mathbb{R}^2\setminus D} \tfrac{1}{2}\theta|\nabla w|^2 - \theta\lambda_* w - \int_{\partial D} (\partial_\nu \psi_d) w$$

The objective is convex in w and linear in θ, so convex duality applies (at least formally). Swapping $\max_\theta$ and $\min_w$ and evaluating $\max_\theta$ by hand gives

$$\max_{\int \theta(x)=\text{const}} \min_{w} \int_{\mathbb{R}^2\setminus D} \tfrac{1}{2}\theta|\nabla w|^2 - \theta\lambda_* w - \int_{\partial D} (\partial_\nu \psi_d) w$$
$$= \min_{w} \int_{\mathbb{R}^2\setminus D} \tfrac{1}{2}(|\nabla w|^2 - \lambda_* w - k)_+ - \int_{\partial D} (\partial_\nu \psi_d) w$$

for some constant k (a Lagrange multiplier for the area constraint).

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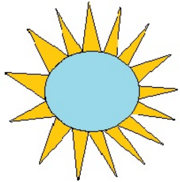

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Conclusions

Wrapping up

- The ENZ limit involves divergence-form operators $\nabla \cdot (a(x)\nabla u)$ where $a(x) = 1/\delta \to \infty$ in the ENZ region.
- Perturbation theory still applies, when done right; everything is analytic in δ.
- Leading-order corrections explain robustness of ENZ-based designs wrt (a) losses, and (b) variation of the frequency.
- The ENZ-based resonator presents an interesting optimal design problem.

Looking ahead: can something similar be done in 3D?

- Since $\nabla \times H = i\omega\varepsilon E$ and $\nabla \times E = -i\omega\mu H$, H is only curl-free in the ENZ region.
- The physics literature does include 3D devices, including 3D resonators a bit like the 2D example. We're looking at them.

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