

Transverse Magnetic ENZ Resonators: Robustness and Optimal Shape Design

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Abstract

We study certain “geometric-invariant resonant cavities” introduced by Liberal, Mahmoud, and Engheta in a 2016 Nature Communications paper. They are cylindrical devices modeled using the transverse magnetic reduction of Maxwell’s equations, so the mathematics is two-dimensional. The cross-section consists of a dielectric inclusion surrounded by an “epsilon-near-zero” (ENZ) shell. When the shell has just the right area, its interaction with the inclusion produces a resonance. Mathematically, the resonance is a nontrivial solution of a 2D divergence-form Helmholtz equation $\nabla \cdot (\varepsilon^{-1}(\mathbf{x}, \omega) \nabla \mathbf{u}) + \omega^2 \mu \mathbf{u} = \mathbf{0}$, where $\varepsilon(\mathbf{x}, \omega)$ is the (complex-valued) dielectric permittivity, ω is the frequency, μ is the magnetic permeability, and a homogeneous Neumann condition is imposed at the outer boundary of the shell. This is a nonlinear eigenvalue problem, since ε depends on ω . Use of an ENZ material in the shell means that $\varepsilon(\mathbf{x}, \omega)$ is nearly zero there, so the PDE is rather singular. Working with a Lorentz model for the dispersion of the ENZ material, we put the discussion of Liberal et. al. on a sound foundation by proving the existence of the anticipated resonance when the loss parameter of the Lorentz model is sufficiently small. Our analysis is perturbative in character, using the implicit function theorem despite the apparently singular form of the PDE. While the existence of the resonance depends only on the area of the ENZ shell, its quality (that is, the rate at which the resonance decays) depends on the shape of the shell. It is therefore natural to consider an associated optimal design problem: what shape shell gives the slowest-decaying resonance? We prove that if the dielectric inclusion is a ball then the optimal shell is a concentric annulus. For an inclusion of any shape, we study a convex relaxation of the design problem using tools from convex duality. Finally, we discuss the conjecture that our relaxed problem amounts to considering homogenization-like limits of nearly optimal designs.

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1 Introduction

This paper is motivated by a 2016 article by Liberal et al, which discusses how epsilon-near-zero (ENZ) materials can be used to design “geometry-invariant resonant cavities” [16]. We focus on a class of examples involving the transverse magnetic reduction of the time-harmonic Maxwell system, obtained by taking $H = (0, 0, u(x_1, x_2))$ and $E = \frac{1}{i\omega\varepsilon}(-\partial_2 u, \partial_1 u, 0)$ in

$$\nabla \times H = -i\omega\varepsilon(x)E, \quad \nabla \times E = i\omega\mu(x)H. \quad (1.1)$$

Thus we shall be working with the Helmholtz equation

$$\nabla \cdot \left(\frac{1}{\varepsilon(x)} \nabla u \right) + \omega^2 \mu(x) u = 0 \quad (1.2)$$

in a bounded two-dimensional domain Ω . Here ω is the frequency, and $\varepsilon = \varepsilon(x_1, x_2)$, $\mu = \mu(x_1, x_2)$ are the dielectric permittivity and magnetic permeability at this frequency.

It is easy to see from (1.2) what is special about ENZ materials in the transverse-magnetic setting. Indeed, if $\varepsilon(x)$ is near zero in some “ENZ region,” then $\frac{1}{\varepsilon(x)} \nabla u$ can avoid being large only by ∇u being small in this region. In the limit as $\varepsilon \rightarrow 0$ in the ENZ region, we are not solving a PDE there but rather choosing a constant value for u . While the solution of a PDE depends sensitively on its domain and coefficients, the constant value of u in the ENZ region should be much less sensitive. In fact, in many settings it is only the *area* of the ENZ region that matters (to leading order, as $\varepsilon \rightarrow 0$ in the ENZ region). This effect has been used, for example, to design entirely new types of waveguides [21; 22; 23]; for recent reviews of these and other applications, see [14; 19].

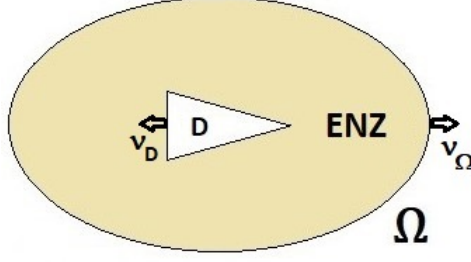


Fig. 1 Our resonator consists of a region D in which $\varepsilon = \varepsilon_0 \varepsilon_D(\omega)$ surrounded by a shell $\Omega \setminus \overline{D}$ in which $\varepsilon = \varepsilon_0 \varepsilon_{\text{ENZ}}(\omega)$. The material in the shell is ENZ, whereas D is occupied by an ordinary dielectric.

We now specify more precisely the PDE problem considered in this paper. The Helmholtz equation (1.2) will be solved in a bounded domain $\Omega \subset \mathbb{R}^2$ with a core-and-shell structure: it consists of a region $D \subset \Omega$ containing an ordinary dielectric, surrounded by a shell $\Omega \setminus D$ containing an ENZ material (see Figure 1). At the outer boundary $\partial\Omega$ we take $\partial u / \partial \nu_\Omega = 0$. (In the language of the underlying Maxwell system, the outer boundary is a perfect electric conductor.) Following [16], we shall ignore the spatial and frequency dependence of μ , since it is negligible in the intended applications; thus we set $\mu(x) = \mu_0$ to be the permeability of free space. The dielectric permittivity ε is constant in each material:

$$\varepsilon(x) = \begin{cases} \varepsilon_0 \varepsilon_D(\omega) & \text{in } D \\ \varepsilon_0 \varepsilon_{\text{ENZ}}(\omega) & \text{in } \Omega \setminus \overline{D} \end{cases} \quad (1.3)$$

where ε_0 is the permittivity of free space. While our method is more general, we shall use a *Lorentz model* for the ENZ material:

$$\varepsilon_{\text{ENZ}}(\omega) = \varepsilon_\infty \left(1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma} \right) \quad (1.4)$$

Here ε_∞ , ω_0 , ω_p and γ are nonnegative real numbers. Notice that in the lossless case $\gamma = 0$ this function vanishes when $\omega = \omega_* := \sqrt{\omega_p^2 + \omega_0^2}$; the resonant frequency of our ENZ-based resonator will be very near this “ENZ frequency.” As for ε_D : following [16], we shall ignore losses there, taking $\varepsilon_D(\omega)$ to be real-valued and positive for real-valued ω near ω_p .

With the preceding conventions, and writing $c = 1/\sqrt{\varepsilon_0\mu_0}$ for the speed of light, the Helmholtz equation (1.2) becomes

$$\nabla \cdot \left(\frac{1}{\varepsilon_D(\omega)} \nabla u \right) + \omega^2 c^{-2} u = 0 \quad \text{in } D \text{ and} \quad (1.5)$$

$$\nabla \cdot \left(\frac{1}{\varepsilon_{\text{ENZ}}(\omega)} \nabla u \right) + \omega^2 c^{-2} u = 0 \quad \text{in } \Omega \setminus \overline{D} \quad (1.6)$$

with the understanding that u and $\frac{1}{\varepsilon}\nabla u \cdot \nu_D$ are continuous at ∂D , and that u satisfies $\partial u / \partial \nu_\Omega = 0$ at $\partial\Omega$. Following [16], we shall refer to a nontrivial solution as a *resonance*. It should be noted, however, that when the loss parameter γ is positive ε_{ENZ} is complex, so the resonance u and the resonant frequency ω will also be complex. Since the time-harmonic Maxwell equations are obtained by considering electric and magnetic fields of the form $e^{-i\omega t}E(x)$ and $e^{-i\omega t}H(x)$, and since physical solutions should decay in time, we expect (and we will find) that in the presence of loss, the imaginary part of ω is negative.

While the preceding discussion is accurate, it ignores an important feature of our analysis. Indeed, in discussing the Lorentz model (1.4) we wrote $\varepsilon_{\text{ENZ}} = \varepsilon_{\text{ENZ}}(\omega)$, treating the constants ε_∞ , ω_0 , ω_p , and γ as being fixed. Actually, the dependence of ε_{ENZ} on the loss parameter γ is crucial to our analysis. In fact, when we prove the existence of a resonance in Section 3, our main tool is perturbation theory in γ , and the resonant frequency is a function of γ . When the dependence of ε_{ENZ} on γ is important, we shall write $\varepsilon_{\text{ENZ}}(\omega, \gamma)$ rather than $\varepsilon_{\text{ENZ}}(\omega)$ for the Lorentz model (1.4) (see for example equation (1.9) below).

Equations (1.5)–(1.6) are not a conventional eigenvalue problem, since ε_D and ε_{ENZ} depend on ω . The fundamental insight of [16] in this context was that *there should nevertheless be a solution near the ENZ frequency when γ is small, provided that the area of the ENZ region satisfies a certain consistency condition*. This result is interesting (and potentially useful) because the consistency condition involves *only* the area of the ENZ region. Usually, for a PDE, the existence of a resonance at a given frequency depends sensitively on the geometry of the domain. Our ENZ-based resonator is different: it has a resonance near the ENZ frequency *regardless* of the shape of the ENZ region, provided only that the area of this region is right. Thus, the design of resonators with a given resonant frequency becomes easy (given the availability of a material with $\varepsilon \approx 0$ at that frequency).

The paper [16] uses physical insight to find the condition on the area of the ENZ region, and it uses numerical simulations to confirm that the anticipated resonances exist in many examples. Our work complements its contributions by proving the existence of such resonances and studying their dependence on the ENZ material's loss parameter γ . In particular, we provide a rather complete understanding about how the geometry of the ENZ region influences the rate at which the resonance decays. It is natural to ask how the shape of the ENZ shell can be chosen to minimize the decay rate. When D is a disk, we show that the optimal ENZ shell is a concentric annulus; for more general D , a similarly explicit solution is probably not possible, but we are nevertheless able to estimate the optimal decay rate by considering a certain convex optimization.

Our account has thus far emphasized the physical character of the problem. To communicate the mathematical character of our work, it convenient (and indeed necessary) to consider what happens when we *ignore* the frequency-dependence of ε_D and ε_{ENZ} . After multiplying both equations (1.5)–(1.6) by ε_D , our PDE (1.2) takes the form

$$\begin{aligned} \nabla \cdot \varepsilon_\delta^{-1} \nabla u + \lambda u &= 0 & \text{in } \Omega \\ \partial_{\nu_\Omega} u &= 0 & \text{at } \partial\Omega, \end{aligned} \tag{1.7}$$

with the conventions that $\lambda = \omega^2 c^{-2} \varepsilon_D$ and $\delta = \varepsilon_{\text{ENZ}}/\varepsilon_D$, and the notation

$$\varepsilon_\delta(x) := \begin{cases} \delta & x \in \Omega \setminus \overline{D} \\ 1 & x \in D. \end{cases} \quad (1.8)$$

Since δ is just a parameter, this *is* a linear eigenvalue problem. It appears to be rather singular in its dependence on δ , since the PDE in $\Omega \setminus \overline{D}$ is now $\nabla \cdot (\delta^{-1} \nabla u) + \lambda u = 0$ and we are interested δ near 0. But it can be desingularized by a suitable ansatz, as we shall explain in Section 2. (In $\Omega \setminus \overline{D}$ the ansatz has $u = 1 + \delta f(x)$, so that $\delta^{-1} \nabla u = \nabla f$ is no longer singular.)

When δ is real and positive, it is a basic result about second-order elliptic PDE that (1.7) can have a nontrivial solution (a resonance) only for a discrete set of λ 's, which must be nonnegative. Our main result about (1.7), Theorem 2.1, identifies the (infinite) set of λ 's for which such a result holds even for *complex-valued* δ in a neighborhood of 0; moreover it shows that for each such resonance, $u = u_\delta$ and $\lambda = \lambda_\delta$ are complex analytic in their dependence on δ . (Our results agree with those in [16] concerning the possible values of $\lambda_0 = \lim_{\delta \rightarrow 0} \lambda_\delta$ and $u_0(x) = \lim_{\delta \rightarrow 0} u_\delta(x)$.) Besides proving analyticity, our work gives easy access to the Taylor expansions of u_δ and λ_δ ; in particular, it identifies the asymptotic electric field in the ENZ region (in other words, the limiting value of $\delta^{-1} \nabla u$ in $\Omega \setminus \overline{D}$ as $\delta \rightarrow 0$), and it shows how the shape of the ENZ shell determines the leading-order correction to λ_0 when $\delta \neq 0$ (that is, the value of $\lambda'(0)$).

Let us say a word about the proof of Theorem 2.1. The arguments draw inspiration from those used to study perturbations of eigenvalues in more standard settings. Due to the singular character of our operator, however, we must solve PDE's in D and $\Omega \setminus \overline{D}$ *separately*, rather than ever solving (1.7) in the entire domain Ω . Our analysis begins by showing how the Taylor expansions of u_δ and λ_δ can be determined term-by-term. While analyticity (with respect to δ) can be proved by majorizing the resulting expansion, we pursue a different approach – demonstrating analyticity by an application of the implicit function theorem.

We are not the first to consider operators of the form $\nabla \cdot (\varepsilon_\delta^{-1} \nabla u)$ in which ε_δ takes only the values 1 and δ and the focus is on behavior near $\delta = 0$. This operator and others like it arise, in particular, when considering the effective behavior or band structure of high-contrast composites [3; 5; 4; 10; 8; 9]. Our treatment of (1.7) has some features in common with the work just cited, as we discuss in more detail near the end of this section.

Returning to the physical problem with dispersion and loss, (1.5)–(1.6): the existence of resonances and their analytic dependence on the loss parameter γ follows easily from Theorem 2.1 by an application of the implicit function theorem. Indeed, it suffices to find a complex-valued function $\omega(\gamma)$ such that

$$\lambda_{\varepsilon_{\text{ENZ}}(\omega(\gamma), \gamma)/\varepsilon_D(\omega(\gamma))} = \omega^2(\gamma) c^{-2} \varepsilon_D(\omega(\gamma)) \quad (1.9)$$

and such that $\omega(0)$ is the ENZ frequency (the one where ε_{ENZ} vanishes when $\gamma = 0$). We show in Theorem 3.1 that the implicit function theorem is applicable, and that the leading-order dependence of $\omega(\gamma)$ (that is, $\omega'(0)$) depends on the geometry of the

ENZ region only through $\lambda'(0)$. Also of note: we show that $\omega'(0)$ is purely imaginary. It follows that the frequency where the resonance occurs (the real part of $\omega(\gamma)$) differs very little from the ENZ frequency (the difference is at most of order γ^2).

For an experimentalist creating a resonator using the framework of this paper, the ENZ material to be used in $\Omega \setminus \overline{D}$ would typically be fixed, and therefore the ENZ frequency ω_* (defined by (3.5)) would also be fixed. As mentioned earlier, the experimentalist's choices of D and Ω must satisfy a consistency condition that depends on ω_* . This is discussed in Section 2.1.3, but we summarize the main impact here: (i) while the shape of D is unconstrained, its size must satisfy a certain (open) condition; (ii) once both the ENZ frequency and D are fixed, the consistency condition constrains Ω only by fixing the area of the ENZ region $\Omega \setminus \overline{D}$.

It is natural to ask how the shape of the ENZ region should be chosen to optimize the associated resonance. Since the imaginary part of ω gives the rate at which the resonance decays, this amounts to asking what shape minimizes $|\omega'(0)|$. The analysis just summarized reduces this to asking what shape minimizes $|\lambda'(0)|$. Our results on the function $\lambda(\delta)$ include a variational characterization of this number: it is a constant times

$$\min_{\phi} \int_{\Omega \setminus \overline{D}} \frac{1}{2} |\nabla \phi|^2 - \lambda_0 \phi \, dx + \int_{\partial D} f \phi \, d\mathcal{H}^1 \quad (1.10)$$

for a particular choice of the function f (see (4.3)). Since the minimum value of (1.10) is negative, our optimal design problem takes the form

$$\max_{\Omega} \min_{\phi} \int_{\Omega \setminus \overline{D}} \frac{1}{2} |\nabla \phi|^2 - \lambda_0 \phi \, dx + \int_{\partial D} f \phi \, d\mathcal{H}^1, \quad (1.11)$$

with the understanding that Ω varies over domains that contain D and remain within some fixed region B . The domain Ω can be represented by a function $\chi(x)$, defined on $B \setminus \overline{D}$, which takes the value 1 on $\Omega \setminus \overline{D}$ and 0 outside Ω . With this convention, (1.11) becomes

$$\max_{\chi(x) \in \{0,1\}} \min_{\phi} \int_{B \setminus \overline{D}} \chi(x) \left(\frac{1}{2} |\nabla \phi|^2 - \lambda_0 \phi \right) dx + \int_{\partial D} f \phi \, d\mathcal{H}^1.$$

In the language of structural optimization (see e.g. [1]), this is a *compliance optimization* problem. Such problems are well-understood for mixtures of two nondegenerate materials (that is, when $\chi(x)$ takes two values that are both positive). In the present more degenerate setting, methods from homogenization cannot be applied directly. But taking inspiration from that theory, we show in Section 4 that the value of (1.11) is upper-bounded by the value of the simple-looking convex optimization

$$\min_{\phi} \int_{B \setminus \overline{D}} \left(\frac{1}{2} |\nabla \phi|^2 - \lambda_0 \phi \right)_+ dx + \int_{\partial D} f \phi \, d\mathcal{H}^1. \quad (1.12)$$

Moreover, we argue (though we do not prove) that this bound is actually sharp. When the inclusion D is a ball we can say much more: the optimal Ω is in fact a concentric ball (and the upper bound (1.12) is indeed sharp in this case).

Let us briefly discuss some related work.

- The physics literature includes many papers on devices made using ENZ materials, including quite a few that can be modeled by Helmholtz equations like (1.2). Many of these papers raise issues comparable to those considered in the present work. Our recent paper [13] studied a phenomenon known as photonic doping; it provided a mathematical foundation for and an improved understanding of an application of ENZ materials considered in [17] (see also [22]). That work involved *scattering*, whereas the present work involves *resonance*. Therefore the analysis in this paper is substantially different from that of [13], though there are of course some parallels. In particular, Section 2 of this paper shows how the perturbation theory of eigenvalue problems can be adapted to the ENZ setting, while our earlier paper was concerned instead with the perturbation theory of boundary-value problems.
- As already mentioned earlier, our treatment of (1.7) has some features in common with [3; 5; 4; 10; 8; 9; 13]. Preparing to say more on this topic, we remind the reader that (1.7) is an eigenvalue problem for the divergence-form operator $\nabla \cdot (\varepsilon_\delta^{-1} \nabla u)$, whose coefficient ε_δ is piecewise constant (equal to 1 in D and δ in $\Omega \setminus \overline{D}$). We show in Section 2 that the quantities of interest are complex analytic functions of δ near $\delta = 0$.

For any function of a complex variable δ , there are two rather distinct approaches to proving its analyticity. One is to show that the function is complex differentiable in δ ; this is what we do in Section 2. The other is to identify the function's Taylor expansion then prove its convergence; this is the approach taken in [3; 5; 4; 8; 9; 13], which consider problems closely related to ours. Among these references, the papers by Chen & Lipton and Fortes, Lipton & Shipman have the strongest connections to our setting, since they too consider spectral problems. This work studies the band structure of certain periodic high-contrast composites; thus its physical motivation is quite different from ours. However, the PDEs considered in these papers are closely analogous to (1.7) (except for being solved on a period cell, with a Bloch boundary condition). Therefore it is not surprising that in these papers, as in Section 2, one finds each successive term of the Taylor expansion by considering (separate) PDE problems in two complementary material regions; moreover, the Taylor expansions found in these papers have a character quite similar to ours. (Since the work just discussed concerns the band structure of periodic high-contrast composites, let us also mention an earlier paper [10], which achieves impressive insight by means other than Taylor expansion.)

Rather than majorize the Taylor expansion, our proof of analyticity uses the implicit function theorem to show that the eigenvalue λ_δ and the (suitably normalized) eigenfunction u_δ of (1.7) are complex-differentiable functions of δ near $\delta = 0$. The fact that perturbation theory for (simple) eigenvalues can be done using the implicit function theorem has been understood at least since 1955 [20]. While this approach does not immediately give a radius of analyticity, extensions of that type have been discussed in some settings [11].

- As we explain in Section 4.3, the passage from (1.11) to (1.12) involves considering the possibility that the optimal Ω is a homogenization limit of domains with many small holes. Our optimal design problem can be regularized by including a penalty term involving the *perimeter* of $\Omega \setminus \overline{D}$. It is known that inclusion of such a penalty

prevents homogenization (see e.g. [2]). However, if the unpenalized optimization requires homogenization then the solution of the penalized problem will depend strongly on the presence and strength of the penalization. Therefore we do not consider the use of perimeter penalization in the present work.

We close this Introduction by summarizing the organization of the paper. Section 2 contains our study of the PDE (1.7). It is the longest section, since much of our success lies in finding a convenient way to desingularize the problem. Section 3 combines the results of Section 2 with the implicit function theorem to show the existence of a resonance near the ENZ frequency, and to consider the effects of dispersion and loss. Finally, Section 4 presents our results on the optimal design problem (choosing the shape of the ENZ region to minimize the effect of loss).

2 Analysis without dispersion

In this section we study the eigenvalue problem (1.7). Our main result is the existence of an eigenfunction u_δ with eigenvalue λ_δ , both depending complex-analytically on δ in a neighborhood of 0, provided that $\lambda_0 = \lim_{\delta \rightarrow 0} \lambda_\delta$ satisfies a certain consistency condition. Our proof shows in addition that λ_δ is a *simple* eigenvalue, in other words its eigenspace is one-dimensional.

We start, in Section 2.1, with some preliminaries and a full statement of the result. Then we show, in Sections 2.2 – 2.3, how the Taylor expansions of u_δ and λ_δ can be determined term-by-term if one assumes analyticity. Finally, in Section 2.4 we use the implicit function theorem to prove the existence of u_δ and λ_δ depending analytically on δ .

Our analysis shows, roughly speaking, that the perturbation theory of eigenvalues and eigenfunctions can be applied to the singular-looking operator $\nabla \cdot \varepsilon_\delta^{-1}(x) \nabla$ with estimates that are uniform in δ (and that $\delta = 0$ is a removable singularity).

2.1 Preliminaries and a statement of our result about u_δ and λ_δ

As discussed in the Introduction, we are interested throughout this paper in a bounded two-dimensional domain Ω with a subset D (see Figure 1). Both domains are assumed to be Lipschitz (that is, their boundaries are locally the graphs of Lipschitz functions) and connected, and \overline{D} does not touch $\partial\Omega$. We also assume that D is simply connected, so that the “ENZ region” $\Omega \setminus \overline{D}$ is a connected set which can be viewed as a shell surrounding D . While the Ω shown in Figure 1 is simply connected, we do not assume this; rather, $\Omega \setminus \overline{D}$ can have one or more holes – in which case the boundary condition $\partial_{\nu_\Omega} u = 0$ in (1.7) applies at the boundary of each hole.

2.1.1 The function ψ_{d,λ_0} ; a normalization; and the consistency condition

It is natural to begin by finding the Taylor expansion of u_δ and λ_δ , assuming existence and analyticity. As a reminder, our goal is to solve

$$\begin{aligned} \nabla \cdot \frac{1}{\varepsilon_\delta} \nabla u_\delta + \lambda_\delta u_\delta &= 0 \quad \text{in } \Omega \\ \partial_{\nu_\Omega} u_\delta &= 0 \quad \text{at } \partial\Omega, \end{aligned} \quad (2.1)$$

where $\varepsilon_\delta(x) := 1$ for $x \in D$ and $\varepsilon_\delta(x) = \delta$ for $x \in \Omega \setminus \overline{D}$. Proceeding formally for the moment, we seek a solution of the form

$$\lambda_\delta = \lambda_0 + \delta\lambda_1 + \delta^2\lambda_2 + \dots \quad (2.2)$$

and

$$u_\delta(x) := \begin{cases} 1 + \delta\phi_1 + \delta^2\phi_2 + \dots & \text{if } x \in \Omega \setminus \overline{D} \\ \psi_0 + \delta\psi_1 + \delta^2\psi_2 + \dots & \text{if } x \in D. \end{cases} \quad (2.3)$$

This should, of course, not be possible for all choices of λ_0 ; the condition that determines the permissible values of λ_0 will be given presently (see (2.9)).

The expansion of u_δ begins with 1 in $\Omega \setminus \overline{D}$ because (as discussed in the Introduction) we expect u_δ to be constant to leading order in $\Omega \setminus \overline{D}$. There is no loss of generality taking the leading-order constant to be 1, since multiplying an eigenfunction by a constant gives another eigenfunction. But this normalization only affects the leading-order term, whereas to fix u_δ we need a condition that applies to all orders in δ . It is convenient to use the normalization

$$\int_{\Omega} u_\delta(x) u_0(x) dx = \int_{\Omega} u_0^2 dx = |\Omega \setminus \overline{D}| + \int_D \psi_0^2 dx, \quad (2.4)$$

where $u_0 = \lim_{\delta \rightarrow 0} u_\delta$ denotes the leading-order term of (2.3),

$$u_0(x) = \begin{cases} 1 & x \in \Omega \setminus \overline{D} \\ \psi_0 & x \in D. \end{cases} \quad (2.5)$$

When we substitute the expansions (2.2)–(2.3) into the PDE (2.1) and focus on the leading-order behavior in D , we see that ψ_0 must solve a Helmholtz equation in D with the Dirichlet boundary condition $\psi_0 = 1$ at ∂D . The solution of this boundary value problem also played a central role in our recent study of photonic doping [13]. To emphasize the connections between that work and this one we will use similar notation here, calling its solution ψ_{d,λ_0} . Thus, we take $\psi_0 = \psi_{d,\lambda_0}$ to be the solution of

$$\begin{aligned} -\Delta \psi_{d,\lambda_0} &= \lambda_0 \psi_{d,\lambda_0} \quad \text{in } D \\ \psi_{d,\lambda_0} &= 1 \quad \text{at } \partial D. \end{aligned} \quad (2.6)$$

We assume here that $\lambda_0 \neq 0$ is real, and that it is not an eigenvalue of $-\Delta$ in D with Dirichlet boundary condition 0. Under these conditions the solution of (2.6) exists and

is unique and real-valued. Since we have only assumed that D is a Lipschitz domain, ψ_{d,λ_0} is in $H_{loc}^2(D) \cap H^1(D)$, which is enough for our purposes. (In [13] the subscript d stood for “dopant;” here it is just a reminder that ψ_{d,λ_0} depends on both D and λ_0 .)

We note for future reference that with the substitution $\psi_0 = \psi_{d,\lambda_0}$, our normalization (2.4) has become

$$\int_{\Omega} u_{\delta}(x) u_0(x) dx = |\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2 dx. \quad (2.7)$$

Since the eigenvalues of an elliptic operator are discrete, we expect that only certain choices of λ_0 should be acceptable. When we consider the expansion term-by-term in Section 2.2, the condition on λ_0 will emerge as the consistency condition for the existence of ϕ_1 ; therefore we like to call it the *consistency condition*. However the same condition can be derived as follows: it is easy to see from (2.1) that

$$\int_{\Omega} u_{\delta} dx = 0 \quad (2.8)$$

by integrating the PDE over Ω and using the homogeneous Neumann boundary condition (along with the assumption that $\lambda_0 \neq 0$). At leading order this gives

$$|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0} dx = 0. \quad (2.9)$$

We shall discuss the solvability of this condition in Section 2.1.3, but we note here that (i) it requires $\int_D \psi_{d,\lambda_0} dx$ to be negative, and (ii) when this integral is negative, (2.9) simply determines the area of the ENZ region.

We assumed above that λ_0 is real-valued and nonzero. Actually, the consistency condition (2.9) implies that it must be positive. Indeed, using the definition (2.6) of ψ_{d,λ_0} we have

$$\begin{aligned} \int_D |\nabla \psi_{d,\lambda_0}|^2 dx &= \int_D \operatorname{div}(\psi_{d,\lambda_0} \nabla \psi_{d,\lambda_0}) dx - \int_D \psi_{d,\lambda_0} \Delta \psi_{d,\lambda_0} dx \\ &= \int_{\partial D} \partial_{\nu_D} \psi_{d,\lambda_0} d\mathcal{H}^1 + \lambda_0 \int_D \psi_{d,\lambda_0}^2 dx. \end{aligned}$$

But using the PDE again along with the consistency condition we have

$$\int_{\partial D} \partial_{\nu_D} \psi_{d,\lambda_0} d\mathcal{H}^1 = \int_D \Delta \psi_{d,\lambda_0} dx = -\lambda_0 \int_D \psi_{d,\lambda_0} dx = \lambda_0 |\Omega \setminus \overline{D}|.$$

Combining these relations, we conclude that

$$\int_D |\nabla \psi_{d,\lambda_0}|^2 dx = \lambda_0 \left(|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2 dx \right).$$

So λ_0 must be positive, as asserted.

2.1.2 Statement of our theorem on analyticity of u_δ and λ_δ

We are ready to state our result on the existence of eigenvalues and eigenvectors of (2.1) depending analytically on δ .

Theorem 2.1. *Let D and Ω be as discussed at the beginning of Section 2.1 and let λ_0 be a positive real number which (i) is not a Dirichlet eigenvalue of $-\Delta$ in D and (ii) satisfies the consistency condition (2.9). Then for all complex δ in a neighborhood of 0 there exists a simple eigenvalue λ_δ of (2.1) with eigenfunction u_δ such that*

$$\lim_{\delta \rightarrow 0} \lambda_\delta = \lambda_0 \quad \text{and} \quad \lim_{\delta \rightarrow 0} u_\delta = u_0 = \begin{cases} 1 & x \in \Omega \setminus \overline{D} \\ \psi_{d,\lambda_0} & x \in D. \end{cases}$$

Moreover, with the normalization (2.7) the eigenfunction u_δ and its eigenvalue λ_δ are complex analytic functions of δ in a neighborhood of $\delta = 0$.

To be sure the final statement is clear: we will show, in the course of the proof, that the map $\delta \mapsto u_\delta$ is a complex analytic function of δ (near $\delta = 0$) taking values in a suitable Banach space. This is equivalent to the statement that u_δ has a Taylor expansion $u_\delta = u_0 + \delta u_1 + \delta^2 u_2 + \dots$ with a positive radius of convergence (see e.g. [6] or [26]).

2.1.3 On satisfying the consistency condition

Our consistency condition (2.9) involves the function ψ_{d,λ_0} , so its dependence on D is not very explicit. This subsection examines how it can be satisfied, either (a) by choosing D and Ω appropriately with λ_0 held fixed, or (b) by choosing λ_0 appropriately, with D and Ω held fixed. (This discussion is not used in the proof of Theorem 2.1. A reader who is mainly interested in that theorem can skip to Section 2.2.)

We start with a representation formula for ψ_{d,λ_0} in terms of the Dirichlet eigenvalues and eigenfunctions of the domain D (more precisely, the spectrum of $-\Delta$ in $H_0^1(D)$). Let $\{\mu_n\}_{n=1}^\infty$ be the Dirichlet eigenvalues of $-\Delta$, and let $\{\chi_n\}_{n=1}^\infty$ be an associated set of orthonormal eigenfunctions; as usual, the eigenvalues are enumerated in nondecreasing order and repeated according to multiplicity. By expressing the function $\psi_{d,\lambda_0} - 1$ (which vanishes at ∂D) in terms of the eigenfunction basis, one finds by a routine calculation that

$$\psi_{d,\lambda_0} = 1 + \lambda_0 \left(\sum_{n=1}^{\infty} \frac{\int_D \chi_n dx}{\mu_n - \lambda_0} \chi_n \right). \quad (2.10)$$

We see from this formula that ψ_{d,λ_0} depends only on the eigenfunctions for which $\int_D \chi_n dx \neq 0$. The following simple proposition assures us that there are infinitely many of these. (For a more quantitative result – estimating how many of the first n Dirichlet eigenfunctions have nonzero mean – see [25].)

Proposition 2.2. *For any bounded domain $D \subset \mathbb{R}^d$ with Lipschitz boundary, there are infinitely many Dirichlet eigenfunctions χ_n such that $\int_D \chi_n(x) dx \neq 0$.*

Proof. The functions $\{\chi_n\}$ form an orthonormal basis of $L^2(D)$. The constant function 1 is in $L^2(D)$ (since D is bounded), so

$$1 = \sum_{n=1}^{\infty} \left(\int_D \chi_n(x) dx \right) \chi_n,$$

where the series on the right, if infinitely many of terms are nonzero, must be understood in the sense of convergence of L^2 functions. Now, if all but finitely many of the coefficients $\int_D \chi_n(x) dx$ were to vanish then the constant function 1 would be a finite sum of eigenfunctions that all vanish at ∂D . This is not possible, so the proposition is proved. \square

The consistency condition (2.9) involves just the *integral* of ψ_{d,λ_0} , which by (2.10) is

$$\int_D \psi_{d,\lambda_0} = |D| + \lambda_0 \sum_{n=1}^{\infty} \frac{(\int_D \chi_n(x) dx)^2}{\mu_n - \lambda_0}. \quad (2.11)$$

We note that the sum on the right hand side of (2.11) is absolutely convergent. Indeed, each term is finite (since by hypothesis λ_0 is not a Dirichlet eigenvalue), and for all but finitely many terms $\mu_n > \lambda_0$ (since the eigenvalues are ordered and tend to infinity). Since all but finitely many of the terms are positive, the sum converges absolutely.

We turn now to the question how the consistency condition (2.9) can be satisfied by choosing D and Ω appropriately, for any fixed positive λ_0 . As already noted earlier, we need only ask how $\int_D \psi_{d,\lambda_0} dx$ can be made negative, since the consistency condition is then satisfied by choosing the area of $\Omega \setminus \overline{D}$ correctly. For a given domain D , it is of course possible for $\int_D \psi_{d,\lambda_0} dx$ to be positive. However, if the Dirichlet eigenvalues of $-\Delta$ in D are $\{\mu_n\}$, then the Dirichlet eigenvalues of $-\Delta$ in the scaled domain tD are μ_n/t^2 . As t varies, there will be selected values where μ_n/t^2 crosses λ_0 for some eigenvalue μ_n such that $\int \chi_n dx \neq 0$. As this crossing happens, we see from (2.11) that the value of $\int_D \psi_{d,\lambda_0} dx$ jumps from $-\infty$ (as μ_n/t^2 approaches λ_0 from below) to $+\infty$ (as μ_n/t^2 increases past λ_0). As t ranges over the interval between two consecutive crossings, $\int_D \psi_{d,\lambda_0} dx$ takes every real value by the intermediate value theorem. Thus, the scale factor t can easily be chosen so that $\int_D \psi_{d,\lambda_0} dx$ is negative.

Finally, we examine how the consistency condition can be satisfied by choosing λ_0 appropriately when D and Ω are held fixed. Combining (2.9) with (2.11), this amounts to studying the roots of $|\Omega| + f(t) = 0$, where

$$f(t) := t \sum_{n=1}^{\infty} \frac{(\int_D \chi_n)^2}{\mu_n - t}. \quad (2.12)$$

We noted above that this sum converges absolutely provided that t is not an eigenvalue with a nonzero-mean eigenfunction. Differentiating term-by-term gives

$$f'(t) = \sum_{n=1}^{\infty} \frac{\mu_n (\int_D \chi_n)^2}{(\mu_n - t)^2} > 0. \quad (2.13)$$

(This calculation is legitimate, since the differentiated sum again converges absolutely; indeed, for large n its n th term is comparable to that of f .) Remembering that an eigenvalue μ_n participates in these sums only if $\int_D \chi_n dx \neq 0$, it is convenient to let $J = \{m_1, m_2, \dots\}$ be the ordered list of eigenvalues having at least one eigenfunction with nonzero mean (which is infinite, by Proposition 2.2). Then we see from (2.12) – (2.13) that $f(t)$ increases monotonically from $-\infty$ to $+\infty$ on each interval $m_i < t < m_{i+1}$. Thus: each of these intervals contains a unique choice of λ_0 for which the consistency condition holds.

2.2 The leading order terms

We have as yet determined only the zeroth-order terms in the Taylor expansions of λ_δ and u_δ . We turn now to the identification of additional terms. The first few, which are discussed in this section, are used in our proof of Theorem 2.1; briefly, knowing them lets us desingularize the PDE problem, permitting application of the implicit function theorem. The higher-order terms, which we discuss in Section 2.3, are also interesting. Indeed, the process by which the expansion is determined term-by-term is intimately related to our implicit-function-theorem-based proof of Theorem 2.1: the implicit function theorem requires the invertibility of a certain linear operator, whereas our identification of each successive term in the expansion involves inverting this operator. (We note in passing that the higher-order terms can also be used to provide an alternative proof of Theorem 2.1 by directly majorizing the Taylor expansions. For arguments of this type in closely analogous settings see [8; 9].)

Before delving into the details, let us provide a big-picture view of the calculation. Our plan is to substitute the expansions (2.2) and (2.3) into the PDE (2.1) and the normalization (2.7) and expand in powers of δ . The condition that λ_0 must satisfy – (2.9) – will emerge naturally as the consistency condition for the PDE problem (in $\Omega \setminus \overline{D}$) that determines ϕ_1 . When this consistency condition holds, ϕ_1 is determined only up to an additive constant, which we call e_1 . The function ψ_1 solves a different PDE problem (in D), which involves ϕ_1 and λ_1 ; as a result, ψ_1 is initially found in terms of the not-yet-determined parameters e_1 and λ_1 . Finally, e_1 and λ_1 are determined by the normalization condition (2.7) and the consistency condition for the existence of ϕ_2 . The process by which ϕ_j , ψ_j , and λ_j are determined for each successive $j = 2, 3, \dots$ is similar.

As we shall see, each function ϕ_j satisfies a Poisson-type equation in $\Omega \setminus \overline{D}$. The associated consistency condition comes from the fact that if $\Delta\phi = f$ in a domain and $\partial_\nu\phi = g$ at its boundary, then the volume integral of f must equal the boundary integral of g . When the equation is consistent, the solution is determined only up to an additive constant. For this reason, it will be convenient to view each ϕ_j as the sum of a mean-zero function and a constant:

$$\phi_n = \mathring{\phi}_n + e_n, \quad e_n \in \mathbb{R}, \quad \int_{\Omega \setminus \overline{D}} \mathring{\phi}_n dx = 0. \quad (2.14)$$

This decomposition induces one of ψ_j , since (as we'll see) ψ_j solves a linear PDE in D with $\psi_j = \phi_j$ at ∂D . While the form of this decomposition will emerge naturally later, we mention it now as a complement to (2.14):

$$\psi_n = \check{\psi}_n + e_n \psi_{d,\lambda_0} \quad \check{\psi}_n = \check{\phi}_n \quad \text{on } \partial D. \quad (2.15)$$

We turn now to the business of this subsection: identification of the initial terms in the expansions. We have, of course, already chosen the order-one terms in the expansion of u_δ :

$$\begin{aligned} \phi_0(x) &:= 1 & \text{for } x \in \Omega \setminus \overline{D}, \\ \psi_0(x) &:= \psi_{d,\lambda_0}(x) & \text{for } x \in D, \end{aligned}$$

Plugging the expansions into the PDE (2.1), at order one in the ENZ region we get a PDE problem for ϕ_1 :

$$\begin{aligned} -\Delta \phi_1 &= \lambda_0 & \text{in } \Omega \setminus \overline{D} \\ \partial_\nu \phi_1 &= 0 & \text{on } \partial\Omega \\ \partial_\nu \phi_1 &= \partial_\nu \psi_{d,\lambda_0} & \text{on } \partial D. \end{aligned} \quad (2.16)$$

Existence requires a consistency condition. Recalling that ν_D denotes the unit normal to ∂D *pointing out of* D , the consistency condition is

$$\lambda_0 |\Omega \setminus \overline{D}| = \int_{\partial D} \frac{\partial \psi_{d,\lambda_0}}{\partial \nu_D} d\mathcal{H}^1. \quad (2.17)$$

When this holds, the solution exists but it is unique only up to an additive constant. Therefore we decompose

$$\phi_1 = \check{\phi}_1 + e_1, \quad e_1 \in \mathbb{R}, \quad \int_{\Omega \setminus \overline{D}} \check{\phi}_1 dx = 0$$

and recognize that while $\check{\phi}_1$ is uniquely determined, e_1 is still unknown. (We note that $\check{\phi}_1$ is real, since ψ_{d,λ_0} is real; therefore our assumption that e_1 take real values is quite natural.)

The consistency condition (2.17) is equivalent to the condition on λ_0 that we introduced earlier, namely (2.9). Indeed, since

$$\int_{\partial D} \frac{\partial \psi_{d,\lambda_0}}{\partial \nu_D} d\mathcal{H}^1 = \int_D \Delta \psi_{d,\lambda_0} dx = -\lambda_0 \int_D \psi_{d,\lambda_0} dx,$$

(2.17) can be rewritten

$$\lambda_0 |\Omega \setminus \overline{D}| = -\lambda_0 \int_D \psi_{d,\lambda_0} dx,$$

which is equivalent to (2.9) since we always assume $\lambda_0 \neq 0$.

We turn now to the identification of the function ψ_1 and the constants λ_1 and e_1 . Since we have already considered the order-one PDE, both in D (in defining ψ_{d,λ_0}) and in $\Omega \setminus \overline{D}$ (in finding $\check{\phi}_1$), we naturally turn to the order- δ problem in D . It says

$$-\Delta\psi_1 = \lambda_1\psi_{d,\lambda_0} + \lambda_0\psi_1 \quad \text{in } D \quad (2.18)$$

$$\psi_1 = \phi_1 \quad \text{on } \partial D. \quad (2.19)$$

(The boundary condition comes from the fact that u_δ cannot jump across ∂D .) For given ϕ_1 and λ_1 , this boundary value problem has a unique solution (since λ_0 is not a Dirichlet eigenvalue of $-\Delta$ in D). Since the additive constant e_1 in ϕ_1 has not yet been determined, it is convenient to make the dependence of ψ_1 on e_1 more explicit. Therefore we decompose ψ_1 as in (2.15):

$$\psi_1 = \check{\psi}_1 + e_1\psi_{d,\lambda_0}, \quad (2.20)$$

where

$$\begin{aligned} -\Delta\check{\psi}_1 &= \lambda_1\psi_{d,\lambda_0} + \lambda_0\check{\psi}_1 \quad \text{in } D \\ \check{\psi}_1 &= \check{\phi}_1 \quad \text{on } \partial D. \end{aligned} \quad (2.21)$$

Since λ_0 is not a Dirichlet eigenvalue of D , any choice of λ_1 uniquely determines $\check{\psi}_1$.

We must still determine e_1 and λ_1 . For this purpose, we shall use the normalization condition (2.7) and the condition that

$$\int_D \check{\psi}_1 dx = 0. \quad (2.22)$$

Some explanation is in order about the latter. Remember that while our condition on λ_0 was initially obtained by requiring that $\int_\Omega u_\delta dx = 0$ at order one, the same condition emerged above as the consistency condition for existence of ϕ_1 . The status of (2.22) is similar. It is at once

- (a) the order- δ version of the condition that $\int_\Omega u_\delta dx = 0$, and
- (b) the consistency condition for existence of ϕ_2 .

To see (a), we observe that

$$\begin{aligned} \int_{\Omega \setminus \overline{D}} \phi_1 dx + \int_D \psi_1 dx &= e_1|\Omega \setminus \overline{D}| + \int_D (\check{\psi}_1 + e_1\psi_{d,\lambda_0}) dx \\ &= \int_D \check{\psi}_1 dx \end{aligned}$$

using the consistency condition (2.9) in the second line. We postpone the justification of (b) to the end of this subsection, since it requires a bit of calculation and it isn't immediately needed.

We now identify the value of λ_1 . Multiplying both sides of (2.21) by ψ_{d,λ_0} and integrating gives

$$\begin{aligned}
\lambda_1 \int_D \psi_{d,\lambda_0} (\psi_{d,\lambda_0} - 1) dx &= - \int_D (\Delta \psi_1 + \lambda_0 \psi_1) (\psi_{d,\lambda_0} - 1) dx \\
&\stackrel{(2.6), (2.22)}{=} \int_{\partial D} \dot{\phi}_1 \partial_{\nu_D} \psi_{d,\lambda_0} d\mathcal{H}^1 \\
&\stackrel{(2.16)}{=} \int_{\partial D} \dot{\phi}_1 \partial_{\nu_D} \dot{\phi}_1 d\mathcal{H}^1 \\
&\stackrel{(2.16)}{=} - \int_{\Omega \setminus \overline{D}} |\nabla \dot{\phi}_1|^2 dx.
\end{aligned} \tag{2.23}$$

Combining this with (2.9), we conclude that

$$\lambda_1 = - \frac{1}{|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2} \int_{\Omega \setminus \overline{D}} |\nabla \dot{\phi}_1|^2 dx. \tag{2.24}$$

We note that this λ_1 does not depend on the as-yet undetermined constant e_1 .

Finally, we identify the value of e_1 using the order δ term in the expansion of the normalization condition (2.7), which is

$$\int_D \psi_1 \psi_{d,\lambda_0} dx + \int_{\Omega \setminus \overline{D}} \phi_1 = 0.$$

Using (2.20), this is equivalent to

$$\int_D \dot{\psi}_1 \psi_{d,\lambda_0} + e_1 \psi_{d,\lambda_0}^2 dx + e_1 |\Omega \setminus \overline{D}| = 0,$$

so

$$e_1 = - \frac{\int_D \dot{\psi}_1 \psi_{d,\lambda_0} dx}{|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2 dx}. \tag{2.25}$$

We note that this definition is not circular: the right hand side of (2.25) involves $\dot{\psi}_1$, which is defined by (2.21) and which therefore depends on λ_1 . However $\dot{\psi}_1$ is independent of e_1 , since our chosen value of λ_1 – given by (2.24) – is independent of e_1 .

A thoughtful reader might ask: is it really true that $\int_D \dot{\psi}_1 dx = 0$ when λ_1 is given by (2.24) and $\dot{\psi}_1$ is determined by (2.21)? The answer is yes. To see why, we revisit

the calculation (2.23) without assuming that this integral vanishes:

$$\begin{aligned}
\lambda_1 \int_D \psi_{d,\lambda_0} (\psi_{d,\lambda_0} - 1) dx &= - \int_D (\Delta \dot{\psi}_1 + \lambda_0 \dot{\psi}_1) (\psi_{d,\lambda_0} - 1) dx \\
&\stackrel{(2.21),(2.6)}{=} \int_{\partial D} \dot{\phi}_1 \partial_{\nu_D} \psi_{d,\lambda_0} d\mathcal{H}^1 + \lambda_0 \int_D \dot{\psi}_1 dx \\
&\stackrel{(2.16)}{=} - \int_{\Omega \setminus \overline{D}} |\nabla \dot{\phi}_1|^2 dx + \lambda_0 \int_D \dot{\psi}_1 dx.
\end{aligned} \tag{2.26}$$

This amounts to a linear relation between λ_1 and $\int_D \dot{\psi}_1 dx$ (since λ_0 , ψ_{d,λ_0} , and $\dot{\phi}_1$ are by now fixed). Our choice of λ_1 is precisely the one that makes $\int_D \dot{\psi}_1 dx$ vanish.

We note for future reference that the functions ϕ_1 and ψ_1 satisfy the order- δ versions of $\int_{\Omega} u_{\delta} dx = 0$ and our normalization condition (2.7), namely

$$\int_{\Omega \setminus \overline{D}} \phi_1 + \int_D \psi_1 dx = 0. \tag{2.27}$$

and

$$\int_{\Omega \setminus \overline{D}} \phi_1 dx + \int_D \psi_1 \psi_{d,\lambda_0} = 0. \tag{2.28}$$

(Indeed, we found λ_1 and e_1 by assuring these relations.)

We close this subsection by justifying our claim that the condition $\int_D \dot{\psi}_1 dx = 0$ is equivalent to the consistency condition for existence of ϕ_2 . Our starting point is the PDE for ϕ_2 , which is the order- δ PDE in $\Omega \setminus \overline{D}$:

$$\begin{aligned}
-\Delta \dot{\phi}_2 &= \lambda_0 \phi_1 + \lambda_1 \phi_0 && \text{in } \Omega \setminus \overline{D} \\
\partial_{\nu_{\Omega}} \dot{\phi}_2 &= 0 && \text{on } \partial \Omega \\
\partial_{\nu_D} \dot{\phi}_2 &= \partial_{\nu_D} \psi_1 = \partial_{\nu_D} \dot{\psi}_1 + e_1 \partial_{\nu_D} \psi_{d,\lambda_0} && \text{on } \partial D.
\end{aligned}$$

Its consistency condition (remembering that ν_D points outward from D) is $-\int_{\Omega \setminus \overline{D}} \Delta \phi_2 dx = \int_{\partial D} \partial_{\nu_D} \phi_2 d\mathcal{H}^1$, in other words

$$\lambda_0 e_1 |\Omega \setminus \overline{D}| + \lambda_1 |\Omega \setminus \overline{D}| = \int_{\partial D} \partial_{\nu_D} \dot{\psi}_1 + e_1 \partial_{\nu_D} \psi_{d,\lambda_0} d\mathcal{H}^1. \tag{2.29}$$

The right side is equal to

$$\int_D \Delta \dot{\psi}_1 + e_1 \Delta \psi_{d,\lambda_0} dx = - \int_D (\lambda_1 \psi_{d,\lambda_0} + \lambda_0 \dot{\psi}_1) dx - e_1 \int_D \lambda_0 \psi_{d,\lambda_0} dx.$$

Using this along with the consistency condition ($|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0} dx = 0$), (2.29) reduces to

$$\lambda_0 \int_D \dot{\psi}_1 dx = 0,$$

which demonstrates our claim (since $\lambda_0 \neq 0$).

2.3 The higher order terms

In this section we explain how the remaining terms in the expansions for u_δ and λ_δ can be found by an inductive procedure. As noted earlier, it is possible to prove Theorem 2.1 by majorizing the resulting series. However our proof – presented in Section 2.4 – uses a different approach, based on the implicit function theorem. Therefore the material in this section will not be used in the rest of the paper; a reader who is mainly interested in the proof of Theorem 2.1 can skip directly to Section 2.4.

Our procedure is inductive: given

$$\{\phi_j\}_{j=1}^n, \{\lambda_j\}_{j=1}^n, \{\psi_j\}_{j=1}^n, \{e_j\}_{j=1}^n, \quad (2.30)$$

satisfying certain properties, we shall explain how to find ϕ_{n+1} , λ_{n+1} , ψ_{n+1} , and e_{n+1} with the analogous properties at level $n+1$. The base case of the induction will be $j=1$, which was addressed in the previous subsection. Throughout this discussion, we understand that ϕ_j and ψ_j are determined by ϕ_j , λ_j , ψ_j , and e_j via

$$\phi_j := \phi_j + e_j, \quad \psi_j = \psi_j + e_j \psi_{d,\lambda_0}. \quad (2.31)$$

Inductive hypotheses:

- For $j = 1, \dots, n$, the functions ϕ_j and ψ_j satisfy

$$\int_{\Omega \setminus \overline{D}} \phi_j dx = 0 \quad \text{and} \quad \int_D \psi_j dx = 0. \quad (2.32)$$

We note that when ϕ_j has mean zero and λ_0 satisfies the consistency condition (2.9),

$$\int_{\Omega \setminus \overline{D}} \phi_j dx + \int_D \psi_j dx = \int_D \psi_j dx;$$

thus, the condition that ψ_j have mean zero is equivalent to

$$\int_{\Omega \setminus \overline{D}} \phi_j dx + \int_D \psi_j dx = 0, \quad (2.33)$$

which amounts to the condition that $\int_\Omega u_\delta dx = 0$ at order δ^j .

- For $j = 1, \dots, n$ the constant e_j is chosen so that

$$\int_{\Omega \setminus \overline{D}} \phi_j dx + \int_D \psi_j \psi_{d,\lambda_0} dx = 0. \quad (2.34)$$

This is simply our normalization condition (2.7) at order δ^j . Using (2.31), we see that it is equivalent to

$$e_j = -\frac{1}{|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2 dx} \int_D \psi_j \psi_{d,\lambda_0} dx. \quad (2.35)$$

A useful identity arises by combining (2.33) and (2.34): subtracting one from the other gives the orthogonality relation

$$\int_D \psi_j (1 - \psi_{d,\lambda_0}) dx = 0. \quad (2.36)$$

Of course, the functions ϕ_j , ψ_j and the constants e_j and λ_j will be chosen for $j = 1, \dots, n$ so that the associated expansions satisfy our PDE (2.1) to a certain order, and the inductive step (choosing these quantities for $j = n + 1$) will assure that the PDE is satisfied to the next order.

As already noted, the base case $j = 1$ is already in place. Indeed, the functions ϕ_1 , ψ_1 and the constants e_1, λ_1 found in Section 2.2 have the desired properties (see (2.28) and (2.27)).

Induction step: We will determine ϕ_{n+1} using the PDE in the ENZ region at order δ^n ; then we will determine ψ_{n+1} , e_{n+1} , and λ_{n+1} by using the PDE in the region D at order δ^{n+1} combined with the $j = n + 1$ versions of conditions (2.32) and (2.34).

Since our argument uses the entire expansion of u_δ and λ_δ , we take the convention that $\phi_0 = 0$, $e_0 = 1$ so that $\phi_0 = \phi_0 + e_0 = 1$; similarly, we take $\psi_0 = 0$ so that $\psi_0 = \psi_{d,\lambda_0}$.

The function $\phi_{n+1} \in H^1(\Omega \setminus \overline{D})$ is obtained by substituting the expansion into the PDE, then focusing on the equation in $\Omega \setminus \overline{D}$ at order δ^n . This gives the Neumann problem

$$\begin{aligned} -\Delta \phi_{n+1} &= \sum_{k=0}^n \lambda_k \phi_{n-k} && \text{in } \Omega \setminus \overline{D} \\ \partial_{\nu_\Omega} \phi_{n+1} &= 0 && \text{on } \partial\Omega \\ \partial_{\nu_D} \phi_{n+1} &= \partial_{\nu_D} \psi_n && \text{on } \partial D \\ \int_{\Omega \setminus \overline{D}} \phi_{n+1}(x) dx &= 0. \end{aligned} \quad (2.37)$$

For a solution to exist, the integral over $\Omega \setminus \overline{D}$ of the bulk source term must be consistent with the integral over ∂D of $\partial_{\nu_D} \psi_n$. Using the PDE for ψ_n , the boundary integral can be expressed as a bulk integral over D . This leads to the consistency condition

$$\sum_{k=0}^n \lambda_k \left[\int_{\Omega \setminus \overline{D}} \phi_{n-k} dx + \int_D \psi_{n-k} dx \right] = 0, \quad (2.38)$$

which holds thanks to (2.33). Thus the PDE problem (2.37) is consistent, and ϕ_{n+1} is its unique mean-zero solution.

Turning now to the PDE in D , at order δ^{n+1} we find the Dirichlet problem

$$\begin{aligned} -\Delta\psi_{n+1} - \lambda_0\psi_{n+1} &= \sum_{k=1}^{n+1} \lambda_k\psi_{n+1-k} && \text{in } D \\ \psi_{n+1} &= \phi_{n+1} = \mathring{\phi}_{n+1} + e_{n+1}\psi_{d,\lambda_0} && \text{on } \partial D. \end{aligned} \quad (2.39)$$

By linearity (and using the definition of ψ_{d,λ_0}), it suffices to solve

$$\begin{aligned} -\Delta\mathring{\psi}_{n+1} - \lambda_0\mathring{\psi}_{n+1} &= \sum_{k=1}^{n+1} \lambda_k\psi_{n+1-k} && \text{in } D \\ \mathring{\psi}_{n+1} &= \mathring{\phi}_{n+1} && \text{on } \partial D. \end{aligned} \quad (2.40)$$

The solution $\mathring{\psi}_{n+1}$ depends on λ_{n+1} , which is as yet unknown. Its value can be obtained by arguing as we did for $j = 1$ in Section 2.2. Inspired by that calculation, we *define* λ_{n+1} by

$$\lambda_{n+1} := \frac{1}{|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2} \int_{\partial D} \mathring{\phi}_{n+1} \partial_{\nu_D} \psi_{d,\lambda_0} d\mathcal{H}^1, \quad (2.41)$$

which is well-defined, since the right hand side involves only quantities that have already been determined. Since we have now fixed λ_{n+1} , the PDE (2.40) determines $\mathring{\psi}_{n+1}$. We may then choose e_{n+1} by

$$e_{n+1} := -\frac{1}{|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2} \int_D \mathring{\psi}_{n+1} \psi_{d,\lambda_0} dx. \quad (2.42)$$

To complete the induction we must check that our choices for $j = n + 1$ meet the requirements of the inductive hypothesis. To do so, it suffices to check that (2.32) and (2.34) hold for $j = n + 1$. The latter follows immediately from our choice of e_{n+1} . To get the former, we multiply both sides of (2.40) by $(\psi_{d,\lambda_0} - 1)$, remembering that this function vanishes at ∂D . Integrating, using the orthogonality in (2.36), and remembering our convention that $\psi_0 = \psi_{d,\lambda_0}$, this calculation gives

$$\begin{aligned} \lambda_{n+1} \int_D \psi_{d,\lambda_0} (\psi_{d,\lambda_0} - 1) dx &= - \int_D (\Delta\mathring{\psi}_{n+1} + \lambda_0\mathring{\psi}_{n+1})(\psi_{d,\lambda_0} - 1) dx \\ &= \int_{\partial D} \mathring{\psi}_{n+1} \partial_{\nu_D} \psi_{d,\lambda_0} d\mathcal{H}^1 + \lambda_0 \int_D \mathring{\psi}_{n+1} \\ &= \int_{\partial D} \mathring{\phi}_{n+1} \partial_{\nu_D} \psi_{d,\lambda_0} d\mathcal{H}^1 + \lambda_0 \int_D \mathring{\psi}_{n+1}. \end{aligned}$$

Combining this with the definition (2.41) of λ_{n+1} , and remembering that $\int_D \psi_{d,\lambda_0} (\psi_{d,\lambda_0} - 1) dx = \int_D \psi_{d,\lambda}^2 dx + |\Omega \setminus \overline{D}|$, we conclude that

$$\int_D \mathring{\psi}_{n+1} = 0.$$

Since ϕ_{n+1} was chosen from the start to have mean value zero, we have confirmed (2.32) and the induction is complete.

2.4 The proof of Theorem 2.1

Our proof will be based on the implicit function theorem. To get started, we shall “desingularize” our eigenvalue problem (2.1), reformulating it in a way that doesn’t involve dividing by δ . This will be done by using the leading order terms of the expansion.

Since we have assumed very little regularity for ∂D and $\partial\Omega$ – they are merely Lipschitz domains – we cannot expect the second derivatives of u_δ to be in $L^2(\Omega)$. Therefore we must work with a fairly weak solution of the PDE. However, standard elliptic regularity results show that our u_δ is actually a smooth function of x away from the boundaries $\partial\Omega$ and ∂D . If the boundaries are smooth, then u_δ is also smooth up to the boundaries (though it cannot be smooth across ∂D , since ε_δ jumps there).

We now establish some notation and discuss the functional analytic framework we will use. The reader can refer to [18] for proofs of the following facts.

- Given a bounded region $A \subset \mathbb{R}^2$ with Lipschitz continuous boundary (in our setting, A will either be $\Omega \setminus \overline{D}$ or D), let ν_A denote the unit normal vector field that points *out* of A . This normal vector exists at \mathcal{H}^1 –almost every point of the boundary ∂A , by Rademacher’s theorem.
- As usual, $H^1(A)$ denotes (possibly complex-valued) square-integrable functions on A with distributional gradients that are also represented by integration against an L^2 vector field. Functions in $H^1(A)$ have a boundary trace. More precisely, there is a bounded linear operator $\gamma_0 : H^1(A) \rightarrow H^{1/2}(\partial A)$ that is surjective. It has the property that $\gamma_0(f)(x) = f(x)$ for any function $f \in H^1(A) \cap C(\overline{A})$, at \mathcal{H}^1 –almost every $x \in \partial A$. When we want to indicate the dependence of γ_0 on the domain A , we will write $\gamma_{0,A}$.

We shall also use the fact that if ξ is an L^2 vector field defined on a bounded Lipschitz domain A with $\nabla \cdot \xi \in L^2(A)$, then it has a well-defined normal trace $\xi \cdot \nu_A$ in $H^{-1/2}(\partial A)$ (the dual of $H^{1/2}(\partial A)$ using the L^2 inner product). It is defined by the property that for any $u \in H^1(A)$ with $\gamma_0(u) = f$,

$$\langle \xi \cdot \nu_A, f \rangle_{H^{-1/2}(\partial A) \times H^{1/2}(\partial A)} = \int_A (\nabla \cdot \xi)u + \xi \cdot \nabla u \, dx, \quad (2.43)$$

and it satisfies

$$\|\xi \cdot \nu_A\|_{H^{-1/2}(\partial A)} \leq C(\|\xi\|_{L^2(A)} + \|\nabla \cdot \xi\|_{L^2(A)}). \quad (2.44)$$

This is well-known, but we briefly sketch the proof since it is not very explicit in [18]. The property (2.43) determines a well-defined linear functional on $H^{1/2}(\partial A)$ since every $f \in H^{1/2}(\partial A)$ is the boundary trace of some $u \in H^1(A)$; we use here the fact that if $\gamma_0(u_1) = \gamma_0(u_2)$ then $u' = u_1 - u_2$ can be approximated in $H^1(A)$ by compactly supported functions, so $\int_A (\nabla \cdot \xi)u' + \xi \cdot \nabla u' \, dx = 0$. The linear functional defined this

way satisfies (2.44), since for every $f \in H^{1/2}(\partial A)$ there exists u such that $\gamma_0(u) = f$ and $\|u\|_{H^1(A)} \leq C\|f\|_{H^{1/2}(\partial A)}$. We will use (2.43)–(2.44) as follows:

- Let

$$S(A) := \{f \in H^1(A) : \Delta f \in L^2(A)\},$$

where Δf denotes the distributional Laplacian of f . Then there is a bounded linear map (the normal derivative trace) $\gamma_1 : S(A) \rightarrow H^{-1/2}(\partial A)$. It has the property that for any $f \in C^1(\bar{A})$, $\gamma_1(f)(x) = \nu_A \cdot \nabla f(x)$ at \mathcal{H}^1 -almost every $x \in \partial A$. The map γ_1 is surjective, by a straightforward application of the Lax-Milgram lemma. When we want to indicate the dependence of γ_1 on A , we will write $\gamma_{1,A}$.

- There is an integration by parts formula: for any $\theta \in H^{-1/2}(\partial A)$, if $f \in S(A)$ is such that $\gamma_1(f) = \theta$, then for all $g \in H^1(A)$ we have

$$\begin{aligned} \langle \theta, \gamma_0(g) \rangle_{H^{-1/2}(\partial A) \times H^{1/2}(\partial A)} &= \langle \gamma_1(f), \gamma_0(g) \rangle_{H^{-1/2}(\partial A) \times H^{1/2}(\partial A)} \\ &= \int_A (\Delta f)g + \nabla f \cdot \nabla g \, dx. \end{aligned}$$

By a convenient abuse of notation we will denote the left hand side by the more familiar expression $\int_{\partial A} g \partial_{\nu_A} f \, d\mathcal{H}^1$.

- The following version of the divergence theorem is obtained by taking $g = 1$ in the preceding identity:

$$\langle \gamma_1(f), 1 \rangle_{H^{-1/2}(\partial A) \times H^{1/2}(\partial A)} = \int_A \Delta f \, dx.$$

We are now ready for the proof of our main theorem.

Proof of Theorem 2.1. We break up the argument into five steps.

STEP 1: We begin by restating our problem in a form that is amenable to use of the implicit function theorem. To find u_δ and λ_δ , we shall seek functions $f_\delta \in H^1(\Omega \setminus \bar{D})$, and $g_\delta \in H^1(D)$ and a real number μ_δ such that

$$u_\delta := \begin{cases} 1 + \delta f_\delta & x \in \Omega \setminus \bar{D} \\ \psi_{d, \lambda_0} + \delta g_\delta & x \in D \end{cases} \quad (2.45)$$

and

$$\lambda_\delta := \lambda_0 + \delta \mu_\delta \quad (2.46)$$

satisfy (2.1) and the normalization (2.7). Note that in view of our formal expansion we expect

$$f_\delta = \phi_1 + \delta \phi_2 + \dots, \quad g_\delta = \psi_1 + \delta \psi_2 + \dots, \quad \mu_\delta = \lambda_1 + \delta \lambda_2 + \dots,$$

so when $\delta = 0$ we expect

$$f_0 = \phi_1, g_0 = \psi_1, \text{ and } \mu_0 = \lambda_1. \quad (2.47)$$

The point of proceeding this way is that when our PDE (2.1) is written in terms of f_δ , g_δ , and μ_δ , there are no longer any negative powers of δ . (For example, the PDE $\delta^{-1}\Delta u_\delta + \lambda_\delta u_\delta = 0$ in the ENZ region $\Omega \setminus \overline{D}$ becomes $\Delta f_\delta + (\lambda_0 + \delta\mu_\delta)(1 + \delta f_\delta) = 0$.)

To apply the implicit function theorem, we shall break our PDE $\nabla \cdot \varepsilon_\delta^{-1} \nabla u_\delta + \lambda_\delta u_\delta = 0$ into three main statements: (i) the PDE holds in D , (ii) the PDE holds in $\Omega \setminus \overline{D}$, and (iii) the continuity of $\varepsilon_\delta \partial_\nu u_\delta$ at ∂D . (There are of course other conditions: u_δ must be continuous across ∂D ; $\partial_{\nu_\Omega} u_\delta$ must vanish at $\partial\Omega$; and our normalization condition must be imposed. These will be built into our chosen function spaces.)

A first-pass idea for proceeding would be to define a function $F(\delta, \mu, f, g)$ such that our PDE is equivalent to $F(\delta, \mu_\delta, f_\delta, g_\delta) = 0$, then prove existence of $(\mu_\delta, f_\delta, g_\delta)$ by applying the implicit function theorem. Our argument is slightly different, because we need an additional constant c_δ to satisfy a consistency condition for the PDE in $\Omega \setminus \overline{D}$. Therefore we shall

- (a) define a function $F(\delta, \mu, f, g, c)$ such that our PDE is equivalent to $F(\delta, \mu_\delta, f_\delta, g_\delta, 0) = 0$; then we'll
- (b) apply the implicit function theorem to solve $F(\delta, \mu_\delta, f_\delta, g_\delta, c_\delta) = 0$; then finally
- (c) we'll use the specific structure of F to show that this solution has $c_\delta = 0$.

STEP 2: We now make the plan concrete by specifying two Banach spaces X and Y and the function $F : X \rightarrow Y$ that will be used. The space X is a subspace of

$$\tilde{X} := \mathbb{C} \times \mathbb{C} \times S(\Omega \setminus \overline{D}) \times S(D) \times \mathbb{C}$$

defined by

$$X := \left\{ (\delta, \mu, f, g, c) \in \tilde{X} \text{ such that } \gamma_{0, \Omega \setminus \overline{D}}(f) = \gamma_{0, D}(g), \gamma_{1, \Omega \setminus \overline{D}}(f)|_{\partial\Omega} = 0, \right. \\ \left. \int_{\Omega \setminus \overline{D}} f + \int_D g \psi_{d, \lambda_0} = 0 \text{ and } \int_{\Omega \setminus \overline{D}} f + \int_D g = 0 \right\}. \quad (2.48)$$

We note that the restrictions defining X assure that u_δ (determined by f , g , and δ via (2.45)) (i) does not jump across ∂D , (ii) satisfies our homogeneous Neumann condition at $\partial\Omega$, (iii) satisfies our normalization condition (2.7), and (iv) satisfies $\int_\Omega u \, dx = 0$. The space Y is

$$Y := L^2(\Omega \setminus \overline{D}) \times H^{-1/2}(\partial D) \times L^2(D). \quad (2.49)$$

The function F is defined by

$$F(\delta, \mu, f, g, c) := \begin{pmatrix} \Delta f + \lambda_0 + \delta(\mu + f(\lambda_0 + \delta\mu)) + c \\ \partial_{\nu_D} f - \partial_{\nu_D}(\psi_{d, \lambda_0} + \delta g) \\ \Delta g + \lambda_0 g + \mu(\psi_{d, \lambda_0} + \delta g) \end{pmatrix}. \quad (2.50)$$

Lest there be any confusion concerning the middle component: since ν_D points outward from D , $\partial_{\nu_D} f$ is really $-\gamma_{1,\Omega \setminus \overline{D}}(f)$. Similarly, $\partial_{\nu_D}(\psi_{d,\lambda_0} + \delta g)$ is really $\gamma_{1,D}(\psi_{d,\lambda_0} + \delta g)$. Evidently, the middle component of F is the difference between two well-defined elements of $H^{-1/2}(\partial D)$.

STEP 3: We will apply the implicit function theorem to get the existence of $(\mu_\delta, f_\delta, g_\delta, c_\delta)$, depending analytically on δ near $\delta = 0$, with μ_0, f_0 , and g_0 given by (2.47) and $c_0 = 0$. While there is a version of the implicit function theorem in the analytic setting (see e.g. [26]), the more familiar C^1 version (e.g. [6, Theorem 10.2.1]) is sufficient for our purposes. Indeed, it assures the existence of $(\mu_\delta, f_\delta, g_\delta, c_\delta)$ with continuous (complex) derivatives with respect to δ . We may then appeal to the fact that such functions are complex analytic (see e.g. [6, Theorem 9.10.1]). It is of course crucial that

$$F(0, \mu_0, f_0, g_0, 0) = 0;$$

our choices (2.47) do have this property (see Sections 2.1 and 2.2).

Since our goal is to solve $F(\delta, z_\delta) = 0$ near $\delta = 0$ with $z = (\mu, f, g, c)$, we must check that (i) F is C^1 , and that (ii) the partial differential of F with respect to z is invertible at $(0, z_0)$ with $z_0 = (\mu_0, f_0, g_0, 0)$. For (i), let us express the differential DF at (δ, μ, f, g, c) as a linear map from X to Y :

$$\begin{aligned} DF_{(\delta, \mu, f, g, c)}(\dot{\delta}, \dot{\mu}, \dot{f}, \dot{g}, \dot{c}) &= \frac{d}{dt} \Big|_{t=0} F(\delta + t\dot{\delta}, \mu + t\dot{\mu}, f + t\dot{f}, g + t\dot{g}, c + t\dot{c}) \\ &= \begin{pmatrix} \dot{\delta}(\mu + f(\lambda_0 + 2\delta\mu)) + \dot{\mu}(\delta + \delta^2 f) + \Delta \dot{f} + \dot{f}\delta(\lambda_0 + \delta\mu) + \dot{c} \\ -\dot{\delta}\partial_{\nu_D} g + \partial_{\nu_D} \dot{f} - \delta\partial_{\nu_D} \dot{g} \\ \dot{\delta}\mu g + \dot{\mu}(\psi_{d,\lambda_0} + \delta g) + \Delta \dot{g} + \dot{g}(\lambda_0 + \mu\delta) \end{pmatrix}. \end{aligned} \quad (2.51)$$

It is now straightforward to see that DF depends continuously (as an operator from X to Y) upon $(\delta, \mu, f, g, c) \in X$. The more subtle task is point (ii). Substituting $(\delta, \mu, f, g, c) = (0, \mu_0, g_0, g_0, 0) = (0, z_0)$ in (2.51) and taking $\dot{\delta} = 0$, we see that the operator to be inverted takes the subspace of X defined by $\delta = 0$ to Y , mapping

$$\dot{z} = (\dot{\mu}, \dot{f}, \dot{g}, \dot{c})$$

to

$$D_z F_{(0, z_0)}(\dot{\mu}, \dot{f}, \dot{g}, \dot{c}) = \begin{pmatrix} \Delta \dot{f} + \dot{c} \\ \partial_{\nu_D} \dot{f} \\ \Delta \dot{g} + \lambda_0 \dot{g} + \psi_{d,\lambda_0} \dot{\mu} \end{pmatrix}. \quad (2.52)$$

So our task is to prove that for all $p, q, r \in Y$, the linear system

$$\begin{aligned} \Delta \dot{f} + \dot{c} &= p && \text{in } \Omega \setminus \overline{D} \\ \partial_{\nu_D} \dot{f} &= q && \text{on } \partial D \\ \Delta \dot{g} + \lambda_0 \dot{g} + \psi_{d,\lambda_0} \dot{\mu} &= r && \text{in } D \end{aligned} \quad (2.53)$$

has a unique solution $(\dot{\mu}, \dot{f}, \dot{g}, \dot{c})$ in $\mathbb{C} \times S(\Omega \setminus \overline{D}) \times S(D) \times \mathbb{C}$ satisfying

$$\begin{aligned} \gamma_{0,\Omega \setminus \overline{D}}(\dot{f}) &= \gamma_{0,D}(\dot{g}), \quad \gamma_{1,\Omega \setminus \overline{D}}(\dot{f})|_{\partial\Omega} = 0, \\ \int_{\Omega \setminus \overline{D}} \dot{f} + \int_D \dot{g} \psi_{d,\lambda_0} &= 0 \quad \text{and} \quad \int_{\Omega \setminus \overline{D}} \dot{f} + \int_D \dot{g} = 0, \end{aligned}$$

and that the solution operator (the map taking (p, q, r) to $(\dot{\mu}, \dot{f}, \dot{g}, \dot{c})$) is a bounded linear map from Y to $\mathbb{C} \times S(\Omega \setminus \overline{D}) \times S(D) \times \mathbb{C}$.

The execution of this task is, of course, very similar to the method by which we found λ_2 , ϕ_2 , and ψ_2 in Section 2.3. We begin by considering the first two equations in (2.53), which give a PDE for \dot{f} in the ENZ region $\Omega \setminus \overline{D}$ with a Neumann boundary condition. For a solution to exist, the consistency condition

$$-\int_{\partial D} q d\mathcal{H}^1 + \dot{c} |\Omega \setminus \overline{D}| = \int_{\Omega \setminus \overline{D}} p dx$$

must hold; therefore the solution has

$$\dot{c} = \frac{1}{|\Omega \setminus \overline{D}|} \left(\int_{\Omega \setminus \overline{D}} p dx + \int_{\partial D} q d\mathcal{H}^1 \right),$$

(which is a bounded linear function of p and q in the given norms). With this choice of \dot{c} the function \dot{f} is undetermined up to an additive constant; as usual, we take $\dot{f} = \mathring{f} + e$ where \mathring{f} is the unique mean-value-zero solution of the first two equations in (2.53) and e will be determined later. Notice that linear operator taking $(p, q) \in L^2(\Omega \setminus \overline{D}) \times H^{-1/2}(\partial D)$ to $\mathring{f} \in S(\Omega \setminus \overline{D})$ is bounded.

We turn now to the third equation in (2.53). Remembering that the trace of \dot{g} must match that of \dot{f} at ∂D , we see that it is to be solved with the Dirichlet boundary condition $\dot{g} = \mathring{f}$ at ∂D . Since λ_0 is not a Dirichlet eigenvalue of $-\Delta$ in D , there is a unique solution; moreover it has the form

$$\dot{g} = \mathring{g} + e \psi_{d,\lambda_0}$$

where \mathring{g} solves

$$\Delta \mathring{g} + \lambda_0 \mathring{g} + \psi_{d,\lambda_0} \dot{\mu} = r \quad \text{in } D, \text{ with } \mathring{g} = \mathring{f} \text{ at } \partial D. \quad (2.54)$$

With the benefit of foresight, we choose

$$\dot{\mu} = \frac{1}{|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2} \left[\int_{\partial D} \mathring{f} \partial_{\nu_D} \psi_{d,\lambda_0} + \int_D r (\psi_{d,\lambda_0} - 1) \right] \quad (2.55)$$

and

$$e = -\frac{1}{|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2} \int_D \mathring{g} \psi_{d,\lambda_0}. \quad (2.56)$$

We note that $\dot{\mu}$ is a bounded linear functional of $(p, q, r) \in Y$, and it doesn't depend on e . Moreover, the operator taking $(p, q, r) \in Y$ to $\dot{g} \in S(D)$ is linear and bounded, since \dot{g} solves a Helmholtz-type PDE in D whose source term $r - \dot{\mu}\psi_{d,\lambda_0}$ and Dirichlet data \dot{f} are in $L^2(D)$ and $H^{1/2}(\partial D)$, each depending linearly on $(p, q, r) \in Y$. Finally, since \dot{g} depends linearly on (p, q, r) and is independent of e , our choice of e is a bounded linear functional of $(p, q, r) \in Y$.

To complete the proof that our linear system is invertible, we must show that our choices (2.55) and (2.56) assure the validity of the relations

$$\int_{\Omega \setminus \overline{D}} \dot{f} + \int_D \dot{g} = 0 \quad \text{and} \quad \int_{\Omega \setminus \overline{D}} \dot{f} + \int_D \dot{g}\psi_{d,\lambda_0} = 0. \quad (2.57)$$

To get the first, we multiply the PDE (2.54) by $\psi_{d,\lambda_0} - 1$, integrate over D , integrate by parts, and use the Dirichlet boundary condition to get

$$-\int_{\partial D} \dot{f}(\partial_{\nu_D} \psi_{d,\lambda_0}) d\mathcal{H}^1 - \lambda_0 \int_D \dot{g} + \dot{\mu} \int_D (\psi_{d,\lambda_0}^2 - \psi_{d,\lambda_0}) dx = \int_D r(\psi_{d,\lambda_0} - 1) dx.$$

Since

$$\int_D (\psi_{d,\lambda_0}^2 - \psi_{d,\lambda_0}) dx = |\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2 dx$$

by the crucial consistency condition (2.9), we see that (2.55) is equivalent to

$$\int_D \dot{g} dx = 0.$$

Since $\dot{f} = \dot{f} + e$ and $\dot{g} = \dot{g} + e\psi_{d,\lambda_0}$, we conclude that

$$\int_{\Omega \setminus \overline{D}} \dot{f} + \int_D \dot{g} = e(|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}) = 0,$$

which gives the first equation in (2.57). As for the other, we have

$$\int_{\Omega \setminus \overline{D}} \dot{f} + \int_D \dot{g}\psi_{d,\lambda_0} = e|\Omega \setminus \overline{D}| + \int_D (\dot{g}\psi_{d,\lambda_0} + e\psi_{d,\lambda_0}^2) dx;$$

evidently, our choice of e in (2.56) is exactly the one that makes this vanish.

We conclude, by the implicit function theorem, the existence of $\mu_\delta, f_\delta, g_\delta, c_\delta$ depending analytically on δ in a (complex) neighborhood of 0, such that $F(\delta, \mu_\delta, f_\delta, g_\delta, c_\delta) = 0$.

STEP 4 We now prove, using the specific structure of F , that in fact $c_\delta = 0$. Indeed, using Green's theorem (but not the fact that $F = 0$), we have

$$\int_{\Omega \setminus \overline{D}} \left(\Delta f_\delta + \lambda_0 + \delta(\mu_\delta + f_\delta(\lambda_0 + \delta\mu_\delta)) + c_\delta \right)$$

$$= - \int_{\partial D} \partial_{\nu_D} f_\delta d\mathcal{H}^1 + (\lambda_0 + \delta\mu_\delta)|\Omega \setminus \overline{D}| + \delta(\lambda_0 + \delta\mu_\delta) \int_{\Omega \setminus \overline{D}} f_\delta + c_\delta |\Omega \setminus \overline{D}|. \quad (2.58)$$

Adding and subtracting some terms, the right hand side can be rewritten as

$$\begin{aligned} & \int_{\partial D} \partial_{\nu_D} (\psi_{d,\lambda_0} + \delta g_\delta - f_\delta) d\mathcal{H}^1 - \int_{\partial D} \partial_{\nu_D} (\psi_{d,\lambda_0} + \delta g_\delta) d\mathcal{H}^1 \\ & + (\lambda_0 + \delta\mu_\delta)|\Omega \setminus \overline{D}| + \delta(\lambda_0 + \delta\mu_\delta) \int_{\Omega \setminus \overline{D}} f_\delta + c_\delta |\Omega \setminus \overline{D}|, \end{aligned}$$

which (applying Green's theorem) is the same as

$$\begin{aligned} & \int_{\partial D} \partial_{\nu_D} (\psi_{d,\lambda_0} + \delta g_\delta - f_\delta) d\mathcal{H}^1 - \int_D \Delta(\psi_{d,\lambda_0} + \delta g_\delta) \\ & + (\lambda_0 + \delta\mu_\delta)|\Omega \setminus \overline{D}| + \delta(\lambda_0 + \delta\mu_\delta) \int_{\Omega \setminus \overline{D}} f_\delta + c_\delta |\Omega \setminus \overline{D}|. \end{aligned}$$

Adding and subtracting some terms and using that $\Delta\psi_{d,\lambda_0} + \lambda_0\psi_{d,\lambda_0} = 0$, the preceding expression can be further rewritten as

$$\begin{aligned} & \int_{\partial D} \partial_{\nu_D} (\psi_{d,\lambda_0} + \delta g_\delta - f_\delta) d\mathcal{H}^1 - \delta \int_D (\Delta g_\delta + (\lambda_0 + \delta\mu_\delta)g_\delta + \mu_\delta\psi_{d,\lambda_0}) \\ & + (\lambda_0 + \delta\mu_\delta) \int_D \psi_{d,\lambda_0} + \delta(\lambda_0 + \delta\mu_\delta) \int_D g_\delta + (\lambda_0 + \delta\mu_\delta)|\Omega \setminus \overline{D}| \\ & + \delta(\lambda_0 + \delta\mu_\delta) \int_{\Omega \setminus \overline{D}} f_\delta + c_\delta |\Omega \setminus \overline{D}|. \end{aligned}$$

Using now the fact that $F(\delta, \mu_\delta, f_\delta, g_\delta, c_\delta) = 0$, we conclude that

$$\begin{aligned} & (\lambda_0 + \delta\mu_\delta) \int_D \psi_{d,\lambda_0} + \delta(\lambda_0 + \delta\mu_\delta) \int_D g_\delta + (\lambda_0 + \delta\mu_\delta)|\Omega \setminus \overline{D}| \\ & + \delta(\lambda_0 + \delta\mu_\delta) \int_{\Omega \setminus \overline{D}} f_\delta + c_\delta |\Omega \setminus \overline{D}| = 0. \end{aligned}$$

Making use of the additional relations $\int_D g_\delta + \int_{\Omega \setminus \overline{D}} f_\delta = 0$ and $|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0} = 0$, we finally conclude that $c_\delta |\Omega \setminus \overline{D}| = 0$. Thus $c_\delta = 0$, as asserted.

STEP 5: Remembering that μ_δ , f_δ , and g_δ determine u_δ and λ_δ via (2.45), we have demonstrated the existence of an eigenpair $(u_\delta, \lambda_\delta)$ depending analytically on δ . The only remaining assertion of the theorem is that this is a simple eigenvalue, i.e. that the eigenspace of λ_δ is one-dimensional. This comes directly from the implicit function theorem, which tells us that $z_\delta = (\mu_\delta, f_\delta, g_\delta, c_\delta)$ is the *only* solution of $F(\delta, z) = 0$ near $z_0 = (\mu_0, f_0, g_0, 0)$ when δ is sufficiently small. If the eigenspace of λ_δ were

multidimensional there would be more than one solution of $F(\delta, z_\delta)$ near $(0, z_0)$; so the eigenspace is one-dimensional. \square

3 Accounting for dispersion and loss

As noted in the Introduction, the dielectric permittivity of a material is generally a function of frequency (this is known as *dispersion*) and it is complex-valued (since waves decay as they propagate through materials). Some key structural conditions are that

$$\varepsilon(\omega) \text{ is holomorphic in the upper half-plane,} \quad (3.1)$$

$$\varepsilon(-\bar{\omega}) = \bar{\varepsilon}(\omega) \text{ for all } \omega \in \mathbb{C}, \text{ and} \quad (3.2)$$

$$\text{the imaginary part of } \varepsilon(\omega) \text{ is nonnegative when } \omega \text{ is real and positive} \quad (3.3)$$

(see e.g. Section 82 of [15]). The class of all such functions is huge. When considering a particular material, however, a parsimonious framework is needed, and for this purpose the *Lorentz model* is often used. (In particular, [16] uses such a model to simulate silicon carbide as an ENZ material.) It has the form

$$\varepsilon(\omega, \gamma) = \varepsilon_\infty \left(1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma} \right) \quad (3.4)$$

where ε_∞ , ω_p , ω_0 , and γ are nonnegative real numbers. (In discussing the dependence of this function on ω with γ held fixed, we shall sometimes omit the variable γ , writing $\varepsilon(\omega)$ rather than $\varepsilon(\omega, \gamma)$.) Viewed as a function of $\omega \in \mathbb{C}$, this model has two poles in the lower half-plane; to leading order as $\gamma \rightarrow 0$ they are at $-\frac{i}{2}\gamma \pm \omega_0$ (provided $\omega_0 \neq 0$). The Lorentz model is, roughly speaking, the simplest functional form consistent with the general principles (3.1)–(3.3) (though it is sometimes simplified further by taking $\omega_0 = 0$; this is known as the Drude model).

Dispersion is more than just a fact of life – it is in fact the *reason* that ENZ materials exist. This is especially easy to see for the Lorentz model. Indeed, in the lossless limit $\gamma = 0$ there is a unique (real and positive) *ENZ frequency*

$$\omega_* = \sqrt{\omega_p^2 + \omega_0^2} \quad (3.5)$$

such that $\varepsilon(\omega_*) = 0$. The presence of loss regularizes the singularity at $\omega = \omega_0$, but it leaves the picture qualitatively intact: the real part of $\varepsilon(\omega)$ vanishes at a γ -dependent real frequency near ω_* . The imaginary part of $\varepsilon(\omega)$ is of course strictly positive when $\gamma > 0$ and ω is real; however when γ is small it is mainly significant near ω_0 . (See Figure 2.)

The main result in this section, Theorem 3.1, uses a Lorentz model for ε_{ENZ} (though as we discuss in Remark 3.2 our method applies more generally). We do not use a

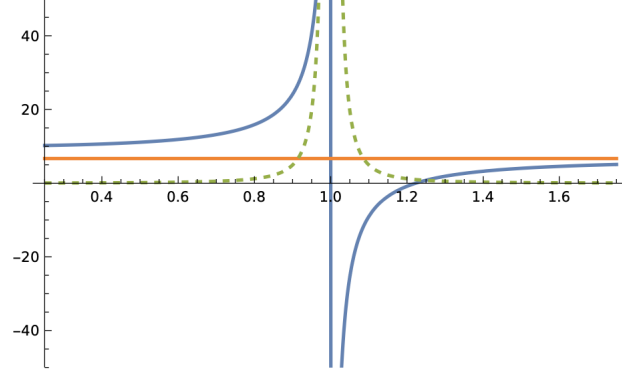


Fig. 2 The Lorentz model $\varepsilon(\omega, \gamma) = \varepsilon_\infty \left(1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma} \right)$, graphed as a function of ω/ω_0 : the solid blue curve is the real part of $\varepsilon(\omega, \gamma)$, while the dotted green curve is the imaginary part. The horizontal orange line shows the value of ε_∞ . This figure was produced using $\varepsilon_\infty = 6.7$, $\omega_p/\omega_0 = 0.7$, and $\gamma/\omega_0 = .006$, consistent with experimental data on silicon carbide near its resonance at frequency $\omega_0 = 2.38 \times 10^{13} \text{sec}^{-1}$ [24]. This material system was used for the simulations in [16].

specific model for ε_D ; rather, we assume only that

$$\varepsilon_D(\omega) \text{ is real-valued when } \omega \text{ is real;} \quad (3.6)$$

$$\varepsilon_D(\omega_*) \text{ is positive, and } \varepsilon_D \text{ is analytic in a neighborhood of } \omega_*; \text{ and} \quad (3.7)$$

$$\text{for real-valued } \omega \text{ near } \omega_*, \frac{d}{d\omega} [\omega^2 \varepsilon_D(\omega)] > 0. \quad (3.8)$$

The first condition says that the material in region D has negligible loss at frequencies near ω_* . (This was assumed in [16].) The second is very routine. The third condition is actually satisfied by any physical material, since when loss is negligible it is known that $\frac{d}{d\omega} [\omega \varepsilon(\omega)] > 0$ when ω is real and positive (see e.g. Section 80 of [15]).

Theorem 3.1. *Let $\varepsilon_{\text{ENZ}} = \varepsilon_{\text{ENZ}}(\omega, \gamma)$ have the form (1.4) for some $\omega_0 \geq 0$ and $\omega_p > 0$ (which will be held fixed), and let ω_* be the associated ENZ frequency (3.5). Suppose further that ε_D satisfies (3.6)–(3.8), that*

$$\lambda_* := \frac{1}{c^2} \omega_*^2 \varepsilon_D(\omega_*) \quad (3.9)$$

is not a Dirichlet eigenvalue of $-\Delta$ in D , and that λ_ satisfies the crucial consistency condition*

$$|\Omega \setminus \overline{D}| + \int_D \psi_{d, \lambda_*} dx = 0 \quad (3.10)$$

(which is (2.9) with λ_0 replaced by λ_). Then there is an analytic function $\omega(\gamma)$ defined in a neighborhood of 0 such that $\omega(0) = \omega_*$ and*

$$\lambda_{\varepsilon_{\text{ENZ}}(\omega(\gamma), \gamma) / \varepsilon_D(\omega(\gamma))} = \omega^2(\gamma) c^{-2} \varepsilon_D(\omega(\gamma)), \quad (3.11)$$

where λ_δ is the function supplied by Theorem 2.1 with λ_0 replaced by λ_ . It follows that (1.5)–(1.6) has a one-dimensional solution space when $\omega = \omega(\gamma)$, spanned by the*

function u_δ provided by Theorem 2.1 with $\delta = \varepsilon_{\text{ENZ}}(\omega(\gamma), \gamma)/\varepsilon_D(\omega(\gamma))$. The value of $\omega'(0)$ can be expressed in terms of

$$a_1 := \partial_\omega \varepsilon_{\text{ENZ}}(\omega_*, 0) \quad (3.12)$$

$$a_2 := \frac{1}{i} \partial_\gamma \varepsilon_{\text{ENZ}}(\omega_*, 0) \quad (3.13)$$

$$a_3 := \partial_\omega (\omega^2 \varepsilon_D(\omega))|_{\omega=\omega_*} \quad (3.14)$$

(all of which are easily seen to be positive real numbers) by

$$\omega'(0) = -i \frac{a_2}{a_1 + a_3 c^{-2} \varepsilon_D(\omega_*) |\lambda'(0)|^{-1}}, \quad (3.15)$$

where $\lambda'(0)$ is given by (2.24).

Before giving the proof, let us discuss a key consequence of this result. When designing a resonator, it is natural to use materials with relatively little loss, so the value γ should be small and $\omega(\gamma) \approx \omega(0) + \omega'(0)\gamma = \omega_* + \omega'(0)\gamma$. Since $\omega'(0)$ is purely imaginary and γ is positive, we see that the real part of $\omega(\gamma)$ (which is, physically speaking, the resonant frequency) is very near the ENZ frequency ω_* (the difference is at most of order γ^2). We also see that the imaginary part of $\omega(\gamma)$ (which controls the quality factor of the resonance – in other words the rate at which it decays) depends on the shape of Ω only through $|\lambda'(0)|$, and that the quality factor is optimized (the decay rate is minimized) by choosing the shape of Ω so that $|\lambda'(0)|$ is as small as possible.

Proof of Theorem 3.1. By the implicit function theorem, it suffices to show that when we calculate $\omega'(0)$ formally by differentiating (3.11), the calculation succeeds (without dividing by 0). Remembering that $\varepsilon_{\text{ENZ}}(\omega_*, 0) = 0$, differentiation with respect to γ at $\gamma = 0$ gives

$$\lambda'(0) \left[\frac{a_1 \omega'(0)}{\varepsilon_D(\omega_*)} + \frac{ia_2}{\varepsilon_D(\omega_*)} \right] = a_3 c^{-2} \omega'(0).$$

Solving for $\omega'(0)$ gives

$$\omega'(0) = -i \frac{a_2}{a_1 - a_3 c^{-2} \varepsilon_D(\omega_*) (\lambda'(0))^{-1}}.$$

Since we know from (2.24) that $\lambda'(0)$ is a negative real number, the preceding expression is equivalent to (3.15). \square

Remark 3.2. While we have assumed, for simplicity, that ε_{ENZ} is given by a Lorentz model, our method is clearly also applicable in other settings. Its key requirements are that (i) $\varepsilon_{\text{ENZ}} = \varepsilon_{\text{ENZ}}(\omega, \gamma)$ be a function of the frequency ω and a single (scalar) loss parameter γ , and that (ii) its partial derivatives at $\gamma = 0$, $\omega = \omega_*$ be such that a_1 and a_2 are positive real numbers. Suppose, for example, that the permittivity of the ENZ material has the form

$$\varepsilon(\omega) = \varepsilon_\infty \left(1 + \sum_{j=1}^N \frac{(\omega_p^j)^2}{(\omega_0^j)^2 - \omega^2 - i\omega\gamma^j} \right)$$

for some (positive, real) constants ω_p^j , ω_0^j , and γ^j , ordered so that $\omega_0^1 < \dots < \omega_0^N$. By the discussion associated with Figure 2, such a material has an ENZ frequency ω_*^j (defined as a root of $\varepsilon(\omega) = 0$ when $\gamma^1, \dots, \gamma^N$ are all set to 0) between ω_0^j and ω_0^{j+1} for each $j = 1, \dots, N-1$. To get a resonance near ω_*^1 (for example), it is natural to use

$$\varepsilon_{\text{ENZ}}(\omega, \gamma) = \varepsilon_\infty \left(1 + \sum_{j=1}^N \frac{(\omega_p^j)^2}{(\omega_0^j)^2 - \omega^2 - i\omega\gamma\hat{\gamma}^j} \right)$$

with $\hat{\gamma}^j = \gamma^j/\gamma^1$. One easily checks that a_1 and a_2 are positive, so our implicit-function-theorem-based argument is applicable. (However our result is local: it gives a resonant frequency $\omega(\gamma)$ for γ near 0. The argument does not show that $\omega(\gamma)$ is defined even for $\gamma = \gamma^1$.)

4 The optimal design problem

Theorem 3.1 proves the existence of a resonance at (complex) frequency $\omega(\gamma)$ when the loss parameter γ is sufficiently close to 0. The theorem's hypotheses involve the area of Ω , but they are otherwise independent of its shape. However, according to eqn. (3.15) the quality of the resonance *does* depend on the shape of Ω . Therefore it is natural to ask how Ω should be chosen so as to *optimize* the resonance. Theorem 3.1 shows that, to leading order in γ , this amounts to asking what shape minimizes $|\lambda'(0)|$.

The function $\lambda(\delta)$ was introduced in Section 2, where our notation was $\lambda(0) = \lambda_0$ and $\lambda'(0) = \lambda_1$. The analysis in Section 3 used a particular choice of λ_0 , which we called λ_* . However our optimal design problem can be considered for any choice of λ_0 . Therefore we revert in this section to the notation of Section 2.

In considering this optimal design problem, we will be holding D and λ_0 fixed. It follows from the consistency condition that $|\Omega \setminus \overline{D}|$ is also fixed. Recalling from (2.24) that

$$\lambda_1 = -\frac{1}{|\Omega \setminus \overline{D}| + \int_D \psi_{d,\lambda_0}^2 dx} \int_D |\nabla \phi_1|^2 dx$$

and observing that the expression in front of the integral is being held fixed, we see that the goal of our optimal design problem is to minimize the value of

$$\frac{1}{2} \int_{\Omega \setminus \overline{D}} |\nabla \phi_1|^2 dx, \quad (4.1)$$

where ϕ_1 solves (2.16), which we repeat for the reader's convenience here:

$$\begin{aligned} -\Delta \phi_1 &= \lambda_0 && \text{in } \Omega \setminus \overline{D} \\ \partial_{\nu_\Omega} \phi_1 &= 0 && \text{on } \partial\Omega \\ \partial_{\nu_D} \phi_1 &= \partial_{\nu_D} \psi_{d,\lambda_0} && \text{on } \partial D. \end{aligned} \quad (4.2)$$

(Since this is a pure Neumann problem, the data must be consistent; this is assured by the consistency condition (2.9), as we showed in Section 2.2. The solution is only unique up to a constant, but the value of (4.1) is independent of this constant.)

It is a standard fact that (4.1) has a variational characterization:

$$-\frac{1}{2} \int_{\Omega \setminus \overline{D}} |\nabla \phi_1|^2 dx = \min_{w \in H^1(\Omega \setminus \overline{D})} \int_{\Omega \setminus \overline{D}} \frac{1}{2} |\nabla w|^2 - \lambda_0 w dx + \int_{\partial D} (\partial_{\nu_D} \psi_{d, \lambda_0}) w d\mathcal{H}^1, \quad (4.3)$$

and that ϕ_1 is optimal for RHS of (4.3). (To explain the sign of the boundary term in the variational principle, we note that ν_D is the *inward* unit normal to $\partial(\Omega \setminus \overline{D})$ at ∂D .) Our optimal design problem can thus be restated as

$$\sup_{\Omega \supset \overline{D}} \inf_{w \in H^1(\Omega \setminus \overline{D})} \int_{\Omega \setminus \overline{D}} \frac{1}{2} |\nabla w|^2 - \lambda_0 w dx + \int_{\partial D} (\partial_{\nu_D} \psi_{d, \lambda_0}) w d\mathcal{H}^1, \quad (4.4)$$

where it is understood that Ω ranges over Lipschitz domains. It might seem that the optimization over Ω should be subject to a constraint on $|\Omega \setminus \overline{D}|$, in view of the consistency condition (2.9). Actually no such constraint is needed, since if the consistency condition is violated then the minimization over w takes the value $-\infty$. (In (4.4) and throughout this section, we write \inf and \sup rather than \min and \max when we do not mean to claim that the optimum is achieved.)

We have two main results on this optimal design problem:

- In Section 4.1 we show that if D is a ball then the optimal Ω is a concentric ball.
- In Section 4.2 we study a convex relaxation of (4.4), which is certainly an upper bound but which is conjecturally equivalent to the unrelaxed problem.

The relationship between our relaxation of (4.4) and the unrelaxed problem is discussed in Section 4.3. As we explain there, our relaxation has a physical interpretation involving homogenization. This use of homogenization is similar to the introduction of composite materials in compliance optimization problems with design-independent loading, as studied for example in [1]. While this interpretation of our relaxation has yet to be justified rigorously for (4.4), it has been fully justified for compliance optimization problems with design-independent loading.

4.1 Optimality of a ball for round D

Theorem 4.1. *If D is a ball, then $|\lambda_1|$ is minimized by taking Ω to be a concentric ball. (Its radius is determined by D and λ_0 through the consistency condition.) Moreover, this optimum is unique: no other Ω can do as well.*

Proof. It suffices to consider the case when D is the unit disk, since the general case is easily reduced to this one by translation and scaling. The function ψ_{d, λ_0} is then radial and quite explicit:

$$\psi_{d, \lambda_0}(r) = \frac{J_0(\lambda_0 r)}{J_0(\lambda_0)}, \quad r \in (0, 1), \quad (4.5)$$

where as usual J_0 is the zeroth order cylindrical Bessel function of the first kind. Since λ_0 is not an eigenvalue of the Laplacian in the unit disc, this is well-defined ($J_0(\lambda_0) \neq 0$).

Let $A_0 = |\Omega \setminus \overline{D}|$ be the area of the ENZ shell. Its value is available from the consistency condition for the existence of ϕ_1 :

$$\lambda_0 A_0 = \int_{\partial D} \partial_{\nu_D} \psi_{d, \lambda_0} d\mathcal{H}^1,$$

which in view of (4.5) gives

$$A_0 = 2\pi \frac{J'_0(\lambda_0)}{J_0(\lambda_0)}.$$

(As noted in earlier sections, we need $\int_{\partial D} \partial_{\nu_D} \psi_{d, \lambda_0} d\mathcal{H}^1 > 0$ in order that the area of $\Omega \setminus \overline{D}$ be positive. This is a condition on λ_0 , which reduces in the present setting to $J'_0(\lambda_0)/J_0(\lambda_0) > 0$.)

Our claim is that the optimal Ω is a ball centered at the origin with area $|D| + |\Omega \setminus \overline{D}| = \pi + A_0$. Let us call this domain Ω_0 ; it is the ball whose radius r_0 satisfies $\pi r_0^2 = \pi + A_0$. The function ϕ_1 associated with Ω_0 is easily made explicit. Since it is clearly radial, we may write $\phi_1 = \phi_1(r)$, so that the boundary value problem (4.2) becomes

$$\begin{aligned} -\phi_1''(r) - \frac{\phi_1'(r)}{r} &= \lambda_0 \quad \text{for } r \in (1, r_0) \\ \phi_1'(r_0) &= 0 \\ \phi_1'(1) &= \psi'_{d, \lambda_0}(1) = \lambda_0 \frac{J'_0(\lambda_0)}{J_0(\lambda_0)}. \end{aligned}$$

The solution is unique up to an additive constant. The general solution of the ODE is $\phi_1(r) = b + c \log r - \lambda_0 \frac{r^2}{4}$, and the boundary condition at $r = r_0$ gives $c = \lambda_0 r_0^2/2$. (The boundary condition at $r = 1$ gives no additional information; it is automatically satisfied, as a consequence of the consistency condition.)

While the constant b is arbitrary, it is convenient to choose it so that $\phi_1(r_0) = 0$. The resulting (now fully determined) function has the property that $\phi_1(r) < 0$ for $1 \leq r < r_0$. (Indeed, ϕ_1 is strictly concave and $\phi_1'(r_0) = 0$, so it is an increasing function on this interval and it vanishes at $r = r_0$.) This implies in particular that

$$\frac{1}{2} |\nabla \phi_1|^2 - \lambda_0 \phi_1 = \frac{1}{2} (\phi_1')^2 - \lambda_0 \phi_1 > 0 \quad \text{for } r \in (1, r_0). \quad (4.6)$$

To demonstrate the optimality of Ω_0 , we shall use the extension of ϕ_1 by 0,

$$\tilde{\phi}_1 = \begin{cases} \phi_1(r) & \text{for } 1 \leq r \leq r_0 \\ 0 & \text{for } r \geq r_0, \end{cases}$$

as a test function in the variational principle that characterizes λ_1 .

Let $\hat{\Omega}$ be a competitor to Ω_0 ; in other words, let $\hat{\Omega} \subset \mathbb{R}^2$ be a bounded, open set with locally Lipschitz boundary that contains \overline{D} and satisfies $|\hat{\Omega} \setminus \overline{D}| = A_0$. If $\hat{\phi}_1$ is

the solution of (4.2) with $\widehat{\Omega}$ in place of Ω , then the variational principle (4.3) gives

$$\begin{aligned}
-\frac{1}{2} \int_{\widehat{\Omega} \setminus \overline{D}} |\nabla \widehat{\phi}|^2 dx &= \int_{\widehat{\Omega} \setminus \overline{D}} \frac{1}{2} |\nabla \widehat{\phi}|^2 - \lambda_0 \widehat{\phi} dx + \int_{\partial D} (\partial_{\nu_D} \psi_{d, \lambda_0}) \widehat{\phi} d\mathcal{H}^1 \\
&= \min_{w \in H^1(\widehat{\Omega} \setminus \overline{D})} \int_{\widehat{\Omega} \setminus \overline{D}} \frac{1}{2} |\nabla w|^2 - \lambda_0 w dx + \int_{\partial D} (\partial_{\nu_D} \psi_{d, \lambda_0}) w d\mathcal{H}^1 \\
&\leq \int_{\widehat{\Omega} \setminus \overline{D}} \frac{1}{2} |\nabla \widetilde{\phi}_1|^2 - \lambda_0 \widetilde{\phi}_1 dx + \int_{\partial D} (\partial_{\nu_D} \psi_{d, \lambda_0}) \widetilde{\phi}_1 d\mathcal{H}^1. \tag{4.7}
\end{aligned}$$

Since $\frac{1}{2} |\nabla \widetilde{\phi}_1|^2 - \lambda_0 \widetilde{\phi}_1$ vanishes outside Ω_0 and is positive in $\Omega_0 \setminus \overline{D}$,

$$\begin{aligned}
\int_{\widehat{\Omega} \setminus \overline{D}} \frac{1}{2} |\nabla \widetilde{\phi}_1|^2 - \lambda_0 \widetilde{\phi}_1 dx &= \int_{(\widehat{\Omega} \setminus \overline{D}) \cap \Omega_0} \frac{1}{2} |\nabla \phi_1|^2 - \lambda_0 \phi_1 dx \\
&\leq \int_{\Omega_0 \setminus \overline{D}} \frac{1}{2} |\nabla \phi_1|^2 - \lambda_0 \phi_1 dx. \tag{4.8}
\end{aligned}$$

Combining this with (4.7) gives

$$\begin{aligned}
-\frac{1}{2} \int_{\widehat{\Omega} \setminus \overline{D}} |\nabla \widehat{\phi}|^2 dx &\leq \int_{\Omega_0 \setminus \overline{D}} \frac{1}{2} |\nabla \phi_1|^2 - \lambda_0 \phi_1 dx + \int_{\partial D} (\partial_{\nu_D} \psi_{d, \lambda_0}) \phi_1 d\mathcal{H}^1 \\
&= -\frac{1}{2} \int_{\Omega_0 \setminus \overline{D}} |\nabla \phi_1|^2 dx
\end{aligned}$$

where in the final step we used (4.3). This confirms the optimality of Ω_0 . To see its uniqueness, we recall that $\frac{1}{2} |\nabla \phi_1|^2 - \lambda_0 \phi_1$ is strictly positive in $\Omega_0 \setminus \overline{D}$. Therefore equality holds in (4.8) only when $\widehat{\Omega} \setminus \overline{D}$ includes the entire domain $\Omega_0 \setminus \overline{D}$. Since both sets have area A_0 , it follows that $\widehat{\Omega} \setminus \overline{D} = \Omega_0 \setminus \overline{D}$, whence $\widehat{\Omega} = \Omega_0$. \square

Remark 4.2. *The preceding argument is simple, but perhaps a bit mysterious. The next section offers a convex-optimization-based perspective on our optimal design problem. In general, for a convex variational problem, if one can guess the optimal test function, then there is usually a simple proof that the guess is right, obtained by using a solution of the dual problem. As we shall show in Proposition 4.4, this is indeed the character of the argument just presented.*

4.2 A convex relaxation

We turn now to the max-min problem (4.4), when D is any simply-connected Lipschitz domain. We start by making some minor adjustments:

- As noted at the beginning of Section 2.1, we do not want to assume that Ω is simply connected. However we want Ω to be a *bounded* domain, and it is therefore natural to introduce the restriction that Ω be a subset of some fixed region B that contains \overline{D} .

- The function $\partial_{\nu_D} \psi_{d,\lambda_0}$ appears in the final term of (4.4), because the PDE for ϕ_1 is driven by this source term at ∂D . However, the analysis in this section applies equally when this function is replaced by any $f \in H^{-1/2}(\partial D)$ such that

$$\int_{\partial D} f d\mathcal{H}^1 > 0. \quad (4.9)$$

To emphasize this, throughout the present section our source term will be f rather than $\partial_{\nu_D} \psi_{d,\lambda_0}$.

- When we replace $\partial_{\nu_D} \psi_{d,\lambda_0}$ by f in the PDE (4.2) defining ϕ_1 , the condition for existence of a solution becomes

$$\lambda_0 |\Omega \setminus \overline{D}| = \int_{\partial D} f d\mathcal{H}^1.$$

Obviously B must be large enough to contain Ω , so we require that

$$|B \setminus \overline{D}| > \frac{1}{\lambda_0} \int_{\partial D} f d\mathcal{H}^1. \quad (4.10)$$

Taking these adjustments into account, our goal is to understand

$$m := \sup_{\substack{\Omega \text{ s.t. } \overline{D} \subset \Omega \subset B}} \inf_{w \in H^1(\Omega \setminus \overline{D})} \int_{\Omega \setminus \overline{D}} \frac{1}{2} |\nabla w|^2 - \lambda_0 w dx + \int_{\partial D} f w d\mathcal{H}^1, \quad (4.11)$$

with the unspoken convention that Ω ranges over Lipschitz domains. It is convenient to write this differently, in terms of the *characteristic function* of Ω , viewed as a function on $B \setminus \overline{D}$ that takes only the values 0 and 1 (outside and inside Ω respectively):

$$m = \sup_{\substack{\chi(x) \in \{0,1\} \text{ for } x \in B \setminus \overline{D} \\ \chi = 1 \text{ at } \partial D}} \inf_{w \in H^1(B \setminus \overline{D})} \int_{B \setminus \overline{D}} \chi(x) \left(\frac{1}{2} |\nabla w|^2 - \lambda_0 w \right) dx + \int_{\partial D} f w d\mathcal{H}^1. \quad (4.12)$$

Our convex relaxation of the optimal design problem is obtained by replacing the characteristic function χ (which takes only the values 0 and 1) by a density θ (which takes any value $0 \leq \theta \leq 1$). Since enlarging the class of test functions in a maximization can only increase the value of the maximum, it is obvious that

$$m \leq m_{\text{rel}} = \sup_{0 \leq \theta(x) \leq 1} \inf_{w \in H^1(B \setminus \overline{D})} \int_{B \setminus \overline{D}} \theta(x) \left(\frac{1}{2} |\nabla w|^2 - \lambda_0 w \right) dx + \int_{\partial D} f w d\mathcal{H}^1. \quad (4.13)$$

There is reason to think that $m = m_{\text{rel}}$, as we shall explain in Section 4.3. For now, however, we focus on the relaxed problem (4.13).

It might seem strange that in formulating the relaxed problem we have kept no remnant of the condition that $\chi = 1$ at ∂D . The reason is that if $\chi = 0$ near a part of ∂D where $f \neq 0$, then the min over w is $-\infty$ (by considering test functions w

supported in the region where $\chi = 0$). So we believe that the value of (4.12) is not changed by dropping the constraint that $\chi = 1$ at ∂D .

Equation (4.13) defines m_{rel} as the sup-inf of

$$L(w, \theta) = \int_{B \setminus \overline{D}} \theta(x) \left(\frac{1}{2} |\nabla w|^2 - \lambda_0 w \right) dx + \int_{\partial D} f w d\mathcal{H}^1 \quad (4.14)$$

We note that L is linear in θ and convex in w , so the inf over w in (4.13) is a concave function of θ and the sup-inf can be viewed as maximizing a concave function of θ subject to the convex constraint $0 \leq \theta(x) \leq 1$. Formally, at least, the associated *dual problem* is obtained by replacing sup-inf by inf-sup:

$$\inf_{w \in H^1(B \setminus \overline{D})} \sup_{0 \leq \theta(x) \leq 1} \int_{B \setminus \overline{D}} \theta(x) \left(\frac{1}{2} |\nabla w|^2 - \lambda_0 w \right) dx + \int_{\partial D} f w d\mathcal{H}^1. \quad (4.15)$$

It is obvious that

$$\sup_{0 \leq \theta(x) \leq 1} \int_{B \setminus \overline{D}} \theta(x) \left(\frac{1}{2} |\nabla w|^2 - \lambda_0 w \right) dx = \int_{B \setminus \overline{D}} \left(\frac{1}{2} |\nabla w|^2 - \lambda_0 w \right)_+ dx$$

with the notation $z_+ = \max\{z, 0\}$, so the formal dual is equivalent to

$$\inf_{w \in H^1(B \setminus \overline{D})} \int_{B \setminus \overline{D}} \left(\frac{1}{2} |\nabla w|^2 - \lambda_0 w \right)_+ dx + \int_{\partial D} f w d\mathcal{H}^1. \quad (4.16)$$

(We will show in due course that this infimum is achieved; but we note here that the functional tends to infinity when $w = c$ is constant and $c \rightarrow \pm\infty$, as an easy consequence of (4.9) and (4.10).)

The following theorem justifies the preceding formal calculation; in particular, it shows that the optimal values of our primal and dual problems are the same, and it proves the existence of an optimal θ for (4.13) and an optimal w for (4.16).

Theorem 4.3. *Let*

$$\mathcal{B} = \{\theta \in L^2(B \setminus \overline{D}) \text{ such that } 0 \leq \theta(x) \leq 1 \text{ a.e.}\},$$

and observe that $L(w, \theta)$ (defined by (4.14)) is well-defined and finite for $\theta \in \mathcal{B}$ and $w \in H^1(B \setminus \overline{D})$. Then

(a) *there is a saddle point $\overline{w} \in H^1(B \setminus \overline{D})$ and $\overline{\theta} \in \mathcal{B}$, in other words a pair such that*

$$L(\overline{w}, \theta) \leq L(\overline{w}, \overline{\theta}) \leq L(w, \overline{\theta})$$

for all $\theta \in \mathcal{B}$ and $w \in H^1(B \setminus \overline{D})$; moreover

(b) *the sup-inf (4.13) and the inf-sup (4.15) have the same value, namely $L(\overline{w}, \overline{\theta})$.*

Proof. We will apply Proposition 2.4 from Chapter 6 of [7]. The overall framework of that chapter involves a functional $L(w, \theta)$ which is defined (and finite) as w and θ range

over closed convex subsets of reflexive Banach spaces. This framework applies to our example, since w ranges over the entire space $H^1(B \setminus \overline{D})$ and θ ranges over \mathcal{B} , which is a closed convex subset of $L^2(B \setminus \overline{D})$. Chapter 6 of [7] needs the additional structural conditions that $\theta \rightarrow L(w, \theta)$ be concave and upper semicontinuous as a function of θ when w is held fixed, and that $w \rightarrow L(w, \theta)$ be convex and lower semicontinuous as a function of w when $\theta \in \mathcal{B}$ is held fixed. Our example meets these requirements.

Proposition 2.4 of [7] has two further hypotheses, namely that

- (i) the constraint set \mathcal{B} is bounded, and
- (ii) there exists $\theta_0 \in \mathcal{B}$ such that

$$\lim_{\|w\| \rightarrow \infty} L(w, \theta_0) = \infty. \quad (4.17)$$

While (i) is valid in our situation, (ii) is not, since it fails when we restrict attention to constant w . To deal with this difficulty, we will proceed in two steps. In the first we restrict θ to lie in the smaller constraint set

$$\tilde{\mathcal{B}} = \mathcal{B} \cap \left\{ \theta \text{ such that } \lambda_0 \int_{B \setminus \overline{D}} \theta \, dx = \int_{\partial D} f \, d\mathcal{H}^1 \right\}, \quad (4.18)$$

which is nonempty by (4.10). For such θ , $L(w, \theta)$ has the property that $L(w, \theta) = L(w + c, \theta)$ for any constant c ; therefore it can be viewed as being defined for all $w \in H^1/\mathbb{R}$. (Here and in the rest of this proof, we use H^1/\mathbb{R} as shorthand for the space $H^1(B \setminus \overline{D})/\mathbb{R}$.) In Step 1 we will show that the saddle point result from [7] applies when θ ranges over $\tilde{\mathcal{B}}$ and w ranges over H^1/\mathbb{R} . Then in Step 2 we will use this result to prove the theorem.

STEP 1. To apply the proposition from [7], it suffices to show that (4.17) is valid when we choose $\theta_0 \in \tilde{\mathcal{B}}$ to have a positive lower bound (for example, we could choose it to be constant), if we view $w \rightarrow L(w, \theta_0)$ as a function on H^1/\mathbb{R} . This is standard; indeed, we may take each equivalence class in H^1/\mathbb{R} to be represented by a function with $\int_{B \setminus \overline{D}} w \, dx = 0$. By Poincaré's inequality, we may take the norm on H^1/\mathbb{R} to be $\|\nabla w\|_{L^2(B \setminus \overline{D})}$. By the trace theorem and Poincaré's inequality, the terms in L that are linear in w are bounded by a constant times $\|w\|$, whereas

$$\int_{B \setminus \overline{D}} \theta_0 |\nabla w|^2 \, dx \geq c \|w\|^2$$

where c is a lower bound for θ_0 . The quadratic term dominates when $\|w\|$ is large enough, so (4.17) holds. With the notation

$$A_0 = \frac{1}{\lambda_0} \int_{\partial D} f \, d\mathcal{H}^1$$

we conclude (applying the result from [7]) that

$$\sup_{\substack{0 \leq \theta \leq 1 \\ \int \theta(x) dx = A_0}} \inf_{w \in H^1/\mathbb{R}} L(w, \theta) = \inf_{w \in H^1/\mathbb{R}} \sup_{\substack{0 \leq \theta \leq 1 \\ \int \theta(x) dx = A_0}} L(w, \theta); \quad (4.19)$$

that there exist $\tilde{\theta}$ (satisfying $0 \leq \tilde{\theta} \leq 1$ and $\int \tilde{\theta} dx = A_0$) and \tilde{w} (in H^1/\mathbb{R}) satisfying

$$L(\tilde{w}, \theta) \leq L(\tilde{w}, \tilde{\theta}) \leq L(w, \tilde{\theta})$$

for all $w \in H^1/\mathbb{R}$ and all $0 \leq \theta \leq 1$ satisfying $\int_{B \setminus \overline{D}} \theta dx = A_0$; and that the value of (4.19) is $L(\tilde{w}, \tilde{\theta})$.

STEP 2. The desired saddle point $(\overline{w}, \overline{\theta})$ will be $(w_1, \tilde{\theta})$, where w_1 is a well-chosen representative of \tilde{w} . To get started, let us examine the relationship between \tilde{w} and $\tilde{\theta}$, using the fact that $\tilde{\theta}$ maximizes $L(\tilde{w}, \theta)$ over all $\theta \in \tilde{B}$. Since $L(w, \theta) = L(w + c, \theta)$ when c is constant and $\theta \in \tilde{B}$, we may work with any representative $w_0 \in H^1(B \setminus \overline{D})$ of \tilde{w} . Evidently, $\tilde{\theta}$ achieves

$$\sup_{\substack{0 \leq \theta \leq 1 \\ \int \theta(x) dx = A_0}} \int_{B \setminus \overline{D}} \theta(x) \left(\frac{1}{2} |\nabla w_0|^2 - \lambda_0 w_0 \right) dx + \int_{\partial D} f w_0 d\mathcal{H}^1. \quad (4.20)$$

Since θ doesn't enter the boundary term, we shall be focusing in what follows on the bulk term. To understand what conclusions we can draw from the optimality of $\tilde{\theta}$, let us assume for a moment that $\frac{1}{2} |\nabla w_0|^2 - \lambda_0 w_0$ has no level sets with positive measure. Then there is a unique $z_0 \in \mathbb{R}$ such that

$$\left| \left\{ x \in B \setminus \overline{D} : \frac{1}{2} |\nabla w_0|^2 - \lambda_0 w_0 > z_0 \right\} \right| = A_0$$

and $\tilde{\theta}$ must be the characteristic function of this set. In general, however, we must allow for the possibility that $\frac{1}{2} |\nabla w_0|^2 - \lambda_0 w_0$ has level sets with positive measure. To deal with this, let

$$g(z) = \left| \left\{ x \in B \setminus \overline{D} : \frac{1}{2} |\nabla w_0|^2 - \lambda_0 w_0 > z \right\} \right|,$$

which is a monotone (but possibly discontinuous) function of $z \in \mathbb{R}$. We can then consider two cases:

- (i) If there exists z_0 such that $g(z_0) = A_0$, then $\tilde{\theta}$ must be the characteristic function of the set where $\frac{1}{2} |\nabla w_0|^2 - \lambda_0 w_0 > z_0$.
- (ii) If no such z_0 exists then there exists z_0 such that $g(z) > A_0$ for $z < z_0$, $g(z) < A_0$ for $z > z_0$, and the set where $\frac{1}{2} |\nabla w_0|^2 - \lambda_0 w_0 = z_0$ has positive measure. In this case $\tilde{\theta}$ must equal 0 where $\frac{1}{2} |\nabla w_0|^2 - \lambda_0 w_0 < z_0$ and it must equal 1 where

$\frac{1}{2}|\nabla w_0|^2 - \lambda_0 w_0 > z_0$. (It is not fully determined by being optimal for (4.20), and it could easily take values between 0 and 1 on the set where $\frac{1}{2}|\nabla w_0|^2 - \lambda_0 w_0 = z_0$; this indeterminacy will not be a problem in what follows.)

Now consider what happens to the preceding calculation when we use a different representative $w_1 = w_0 + c$. The argument applies equally to w_1 , except that the role of z_0 is played by $z_1 = z_0 - \lambda_0 c$, since $\frac{1}{2}|\nabla w_1|^2 - \lambda_0 w_1 = \frac{1}{2}|\nabla w_0|^2 - \lambda_0 w_0 - \lambda_0 c$.

We now choose $c = z_0/\lambda_0$, so that $z_1 = 0$ and

$$\int_{B \setminus \overline{D}} \tilde{\theta} \left(\frac{1}{2}|\nabla w_1|^2 - \lambda_0 w_1 \right) dx = \int_{B \setminus \overline{D}} \left(\frac{1}{2}|\nabla w_1|^2 - \lambda_0 w_1 \right)_+ dx,$$

from which it follows that

$$L(w_1, \tilde{\theta}) \geq L(w_1, \theta) \quad \text{for all } \theta \in \mathcal{B}.$$

We also have

$$L(w_1, \tilde{\theta}) \leq L(w, \tilde{\theta}) \quad \text{for all } w \in H^1(B \setminus \overline{D})$$

since w_1 is a representative of \tilde{w} . In short: $(w_1, \tilde{\theta})$ is a saddle point of L , viewed as a function on $H^1(B \setminus \overline{D}) \times \mathcal{B}$. Thus, we have proved part (a) of the theorem, with $(\bar{w}, \bar{\theta}) = (w_1, \tilde{\theta})$. Part (b) is also clear from the preceding arguments – though it is not really necessary to check, since in general the existence of a saddle point $(\bar{w}, \bar{\theta})$ implies that the sup-inf and inf-sup are equal, and that their common value is $L(\bar{w}, \bar{\theta})$ (see e.g. Proposition 1.2 in Chapter 6 of [7]). \square

Theorem 4.1 showed that when D is a ball and $f = \partial_{\nu_D} \psi_{d, \lambda_0}$, the unique optimal Ω is a concentric ball. It is natural to ask whether uniqueness holds even in the larger class of relaxed designs. The following result provides an affirmative answer – not only when D is a ball, but also for any D such that there exists an optimal (unrelaxed) ENZ shell. In addition, this result and its proof provide a fresh perspective on the argument we used for Theorem 4.1.

Proposition 4.4. *Let $\bar{w} \in H^1(B \setminus \overline{D})$ and $\bar{\theta} \in \mathcal{B}$ be a saddle point for the functional L defined by (4.14). Suppose furthermore that $\bar{\theta}$ solves the unrelaxed optimal design problem – in other words that it is the characteristic function of $\Omega_0 \setminus \overline{D}$ for some connected Lipschitz domain Ω_0 which contains \overline{D} and is compactly contained in B . Then:*

- (i) $\Omega_0 \setminus \overline{D}$ is exactly the subset of $B \setminus \overline{D}$ where $\frac{1}{2}|\nabla \bar{w}|^2 - \lambda_0 \bar{w} > 0$; and
- (ii) for any other saddle point $(\hat{w}, \hat{\theta})$ of L , we have $\hat{\theta} = \bar{\theta}$ and there is a constant c such that $\hat{w} = \bar{w} + c$ in $\Omega_0 \setminus \overline{D}$.

If we assume a little more regularity – specifically, if we assume that Ω_0 is a C^2 domain, and that $\nabla \bar{w}(x)$ is uniformly continuous as x approaches $\partial\Omega_0$ from within Ω_0 – we can say further that

- (iii) $\bar{w} = 0$ at $\partial\Omega_0$.

It follows that the constant c in part (ii) is actually 0, and that \bar{w} satisfies the overdetermined boundary condition

$$\partial_\nu \bar{w} = 0 \text{ and } \bar{w} = 0 \text{ at } \partial\Omega_0. \quad (4.21)$$

Remark 4.5. Our hypothesis that $\nabla \bar{w}(x)$ be uniformly continuous as x approaches $\partial\Omega_0$ from within Ω_0 follows from standard elliptic regularity results if $\partial\Omega_0$ is smooth enough.

Remark 4.6. We saw in Section 4.1 that when D is a ball, a concentric ball with the right area is optimal. The proof used the associated \bar{w} , which vanished at the boundary of the concentric ball. (The PDE that \bar{w} solves in $\Omega_0 \setminus \bar{D}$ determines it only up to an additive constant; however we saw in the proof of Theorem 4.3 why for a saddle point of L we need \bar{w} to vanish – rather than simply being constant – on $\partial\Omega_0$.) It is not surprising that in a shape optimization problem, the associated PDE should satisfy an overdetermined boundary condition. But we wonder whether, for general D , there is really a domain Ω_0 containing \bar{D} for which there exists a solution of $-\Delta w = \lambda_0$ in $\Omega_0 \setminus \bar{D}$ with $\partial_{\nu_D} w = f$ at ∂D and the overdetermined condition (4.21) at $\partial\Omega_0$. If not, then our optimal design problem would have no (sufficiently regular) classical solution, though it always has a relaxed solution.

Proof of Proposition 4.4. We have assumed that Ω_0 is a connected Lipschitz domain, but we have not assumed that it is simply connected. Thus $\Omega_0 \setminus \bar{D}$ is a bounded and connected domain in \mathbb{R}^2 which could have finitely many “holes.”

To get started, we collect some easy observations that follow from $(\bar{w}, \bar{\theta})$ being a saddle point. The first is that $\bar{\theta}$ must actually be in $\tilde{\mathcal{B}}$ (defined by (4.18)), since otherwise $\min_{w \in H^1(B \setminus \bar{D})} L(w, \bar{\theta})$ would be $-\infty$. Our second observation is that $-\Delta \bar{w} = \lambda_0$ in $\Omega_0 \setminus \bar{D}$ with $\partial_\nu \bar{w} = 0$ at $\partial\Omega_0$ and $\partial_{\nu_D} \bar{w} = f$ at ∂D , since \bar{w} minimizes $L(w, \bar{\theta})$ and $\bar{\theta}$ is the characteristic function of $\Omega_0 \setminus \bar{D}$. Our third observation is that $\frac{1}{2}|\nabla \bar{w}|^2 - \lambda_0 \bar{w}$ cannot be constant on a set of positive measure in $\Omega_0 \setminus \bar{D}$, since

$$\Delta \left(\frac{1}{2} |\nabla \bar{w}|^2 - \lambda_0 \bar{w} \right) = |\nabla \nabla w|^2 + \lambda_0^2 > 0.$$

(We note that, by elliptic regularity, that \bar{w} is smooth in the interior of $\Omega_0 \setminus \bar{D}$.) Our fourth observation is that

$$\frac{1}{2} |\nabla \bar{w}|^2 - \lambda_0 \bar{w} \geq 0 \quad \text{in } \Omega_0 \setminus \bar{D}, \text{ and } \quad \frac{1}{2} |\nabla \bar{w}|^2 - \lambda_0 \bar{w} \leq 0 \quad \text{outside of } \Omega_0,$$

since $\bar{\theta}$ maximizes $\int_{B \setminus \bar{D}} \theta \left(\frac{1}{2} |\nabla \bar{w}|^2 - \lambda_0 \bar{w} \right) dx$ over all θ such that $0 \leq \theta(x) \leq 1$.

Assertion (i) of the Proposition is now easy: combining our third and fourth observations, Ω_0 must agree a.e. with the set where $\frac{1}{2} |\nabla \bar{w}|^2 - \lambda_0 \bar{w} > 0$.

For assertion (ii), we argue as we did for Theorem 4.1:

$$L(\hat{w}, \hat{\theta}) \leq L(\bar{w}, \bar{\theta}) \quad (4.22)$$

$$\begin{aligned}
&= \int_{B \setminus \overline{D}} \hat{\theta} \left(\frac{1}{2} |\nabla \overline{w}|^2 - \lambda_0 \overline{w} \right) dx + \int_{\partial D} f \overline{w} d\mathcal{H}^1 \\
&\leq \int_{B \setminus \overline{D}} \bar{\theta} \left(\frac{1}{2} |\nabla \overline{w}|^2 - \lambda_0 \overline{w} \right) dx + \int_{\partial D} f \overline{w} d\mathcal{H}^1 \\
&= L(\overline{w}, \bar{\theta}).
\end{aligned}$$

But the saddle value is unique (see e.g. Proposition 1.2 in Chapter 6 of [7]). Therefore both inequalities in the preceding argument are actually equalities; in particular, $\hat{\theta}$ maximizes $\int_{B \setminus \overline{D}} \theta \left(\frac{1}{2} |\nabla \overline{w}|^2 - \lambda_0 \overline{w} \right) dx$ over all θ such that $0 \leq \theta(x) \leq 1$. Arguing as for part (i), it follows that $\hat{\theta} = 1$ where $\frac{1}{2} |\nabla \overline{w}|^2 - \lambda_0 \overline{w} > 0$. But by the argument of our first observation, $\hat{\theta}$ has the same integral as $\bar{\theta}$. So $\hat{\theta}$ must vanish outside of Ω_0 .

It remains to explain $\overline{w} - \hat{w}$ must be constant in Ω_0 . For this, we combine (4.22) with the fact that $\hat{\theta} = \bar{\theta}$. Substituting $\hat{w} = \overline{w} + (\hat{w} - \overline{w})$ into the fact that $L(\hat{w}, \bar{\theta}) = L(\overline{w}, \bar{\theta})$, expanding the square, and using the stationarity of the functional at \overline{w} , we conclude that $\int_{B \setminus \overline{D}} \bar{\theta} |\nabla \hat{w} - \nabla \overline{w}|^2 dx = 0$. Writing this as $\int_{\Omega_0 \setminus \overline{D}} |\nabla \hat{w} - \nabla \overline{w}|^2 dx = 0$ and using that $\Omega_0 \setminus \overline{D}$ is connected, we conclude that $\hat{w} - \overline{w}$ must be constant on this domain.

Turning now to part (iii): consider any component \mathcal{C} of $\partial \Omega_0$ (which is now assumed to be a finite collection of C^2 curves). Our arguments will be local, in a vicinity of the curve \mathcal{C} . The points to one side belong to $\Omega_0 \setminus \overline{D}$, where \overline{w} satisfies $\frac{1}{2} |\nabla \overline{w}|^2 - \lambda_0 \overline{w} > 0$. Since we have assumed that $\nabla \overline{w}(x)$ is uniformly continuous as x approaches the boundary from $\Omega_0 \setminus \overline{D}$, we can pass to the limit in the inequality and use that $\partial_\nu \overline{w} = 0$ at $\partial \Omega_0$ to conclude that

$$\frac{1}{2} |\partial_s \overline{w}|^2 - \lambda_0 \overline{w} \geq 0 \quad \text{on the chosen component } \mathcal{C}, \quad (4.23)$$

where ∂_s represents the derivative tangent to the boundary.

On the other side of \mathcal{C} we have no PDE for \overline{w} , however we know that

$$\frac{1}{2} |\nabla \overline{w}|^2 - \lambda_0 \overline{w} \leq 0 \quad \text{outside of } \Omega_0. \quad (4.24)$$

We shall use this to show that

$$\frac{1}{2} |\partial_s \overline{w}|^2 - \lambda_0 \overline{w} \leq 0 \quad \text{on the chosen component } \mathcal{C}. \quad (4.25)$$

As a first step, we now show that \overline{w} is uniformly Lipschitz continuous in the complement of Ω_0 . Clearly $\overline{w} \geq 0$ outside of Ω_0 , as a consequence of (4.24). Since $\overline{w} \in H^1(B \setminus \overline{D})$, its L^2 norm is bounded, so using (4.24) once again we see that $\int_{B \setminus \overline{\Omega}_0} |\nabla \overline{w}|^4 dx < \infty$. Since we are in two space dimensions, it follows that \overline{w} uniformly bounded on $B \setminus \overline{\Omega}_0$. Appealing to (4.24) once again, we conclude that

$$|\nabla \overline{w}| \leq M \quad \text{outside } \Omega_0,$$

where M is an upper bound for $\sqrt{2\lambda_0 \overline{w}}$.

Now we combine the bulk inequality (4.24) with the Lipschitz estimate to get (4.25). Since \mathcal{C} is a C^2 curve, we may use tubular coordinates for points in the complement of Ω_0 that lie sufficiently close to \mathcal{C} . We shall use t for the distance to \mathcal{C} , and s for the arclength parameter along a curve at constant distance t . To bound $\partial_s \bar{w}$ at some point $(s_0, 0)$ on \mathcal{C} , we shall estimate the difference quotient $\bar{w}(s_0 + \delta, 0) - \bar{w}(s_0, 0)$ then pass to the limit $\delta \rightarrow 0$. Clearly

$$\begin{aligned} & \bar{w}(s_0 + \delta, 0) - \bar{w}(s_0, 0) \\ &= [\bar{w}(s_0 + \delta, 0) - \bar{w}(s_0 + \delta, t)] + [\bar{w}(s_0 + \delta, t) - \bar{w}(s_0, t)] + [\bar{w}(s_0, t) - \bar{w}(s_0, 0)]. \end{aligned}$$

The first and last terms have magnitude at most Mt . The middle term can be estimated using (4.24) (which for a.e. t holds almost everywhere in s – we naturally restrict our attention to values of t with this property). In fact,

$$\begin{aligned} |\bar{w}(s_0 + \delta, t) - \bar{w}(s_0, t)| &\leq \int_{s_0}^{s_0 + \delta} \partial_s \bar{w}(\sigma, t) d\sigma \\ &\leq \delta^{1/2} \left(\int_{s_0}^{s_0 + \delta} (\partial_s \bar{w})^2(\sigma, t) d\sigma \right)^{1/2} \end{aligned}$$

From (4.24) we have

$$(\partial_s \bar{w})^2(\sigma, t) \leq 2\lambda_0 \bar{w}(\sigma, t) \leq 2\lambda_0 \bar{w}(s_0, 0) + O(|\delta| + |t|),$$

so

$$\int_{s_0}^{s_0 + \delta} (\partial_s \bar{w})^2(\sigma, t) d\sigma \leq \delta [2\lambda_0 \bar{w}(s_0, 0) + O(|\delta| + |t|)].$$

Combining these estimates then sending $t \rightarrow 0$ with δ held fixed, we get

$$|\bar{w}(s_0 + \delta, 0) - \bar{w}(s_0, 0)| \leq \delta (2\lambda_0 \bar{w}(s_0, 0) + O(|\delta|))^{1/2}.$$

Dividing by δ then passing to the limit $\delta \rightarrow 0$, we conclude that

$$|\partial_s \bar{w}(s_0, 0)| \leq (2\lambda_0 \bar{w}(s_0, 0))^{1/2}.$$

Since $(s_0, 0)$ was an arbitrary point on the chosen component \mathcal{C} , this confirms the validity of (4.25). (We note that since $\bar{w} \in H^1(B \setminus \overline{D})$, its traces on $\partial\Omega_0$ taken from inside and outside Ω_0 are the same. So while (4.23) and (4.25) were obtained by taking limits from opposite sides of \mathcal{C} , they estimate the same function on \mathcal{C} .)

Combining (4.23) and (4.25), we have shown that

$$\frac{1}{2} |\partial_s \bar{w}|^2 - \lambda_0 \bar{w} = 0 \quad \text{on the chosen component } \mathcal{C}.$$

To see that this implies $\bar{w} = 0$, we note that since $\bar{w} \geq 0$ on \mathcal{C} , the preceding relation can be rewritten as

$$\partial_s \bar{w} = \pm \sqrt{2\lambda_0 \bar{w}}. \quad (4.26)$$

Now recall our assumption for part (iii) that $\nabla \bar{w}(x)$ is uniformly continuous as x approaches $\partial\Omega_0$ from within the domain Ω_0 . This implies that when viewed as a function on \mathcal{C} , \bar{w} is C^1 . Therefore the \pm sign in (4.26) cannot change at a point where $\bar{w} \neq 0$. If, at some point on \mathcal{C} , the function \bar{w} is strictly positive and (4.26) holds with a plus sign, then \bar{w} must grow as s increases. Similarly, if \bar{w} is strictly positive and (4.26) holds with a minus sign, then \bar{w} must grow as s decreases. Either way we reach a contradiction, since \mathcal{C} is a *closed* curve in the plane, and \bar{w} is a C^1 function on this curve. Since this argument applies to any component of $\partial\Omega_0$, we conclude that $\bar{w} = 0$ on the entirety of $\partial\Omega_0$, and the proof is complete. \square

4.3 The physical meaning of the relaxed problem

In the previous section, our convex relaxation of the optimal design problem was introduced by replacing a maximization over characteristic functions $\chi(x) \in \{0, 1\}$ by one over densities $\theta(x) \in [0, 1]$ (see (4.12) and (4.13)). We believe that the relaxed problem and the original one are in a certain sense equivalent. Precisely: we believe that an optimal θ for the relaxed problem is the weak limit of a maximizing sequence for the original problem. This section explains why we believe this, though we do not have a rigorous proof.

The basic idea is simple. If $\{\chi_k(x)\}_{k=1}^\infty$ is a maximizing sequence of characteristic functions for the original problem (4.12), then it is easy to show the existence of a subsequence converging weakly to some function $\theta(x)$ that takes values in $[0, 1]$. If the domains $\Omega_k = \{x : \chi_k(x) = 1\}$ get increasingly complex – for example, if they are perforated by many small holes – then the weak limit $\theta(x)$ represents the *asymptotic density* of material at x in the limit $k \rightarrow \infty$. The asymptotic performance of Ω_k depends on more than just the density – it is also sensitive to the microstructural geometry. To avoid discussing the microstructure explicitly, it is natural to simply assume that for each x , the microstructure at x is optimal given the density $\theta(x)$. We believe that this is the effect of replacing $\chi(x)(\frac{1}{2}|\nabla w|^2 - \lambda_0 w)$ in (4.12) by $\theta(x)(\frac{1}{2}|\nabla w|^2 - \lambda_0 w)$ in (4.13).

To explain the last statement, we make recourse to the theory of homogenization. For any $\varepsilon > 0$, let $a_k^\varepsilon(x) = \chi_k(x) + \varepsilon(1 - \chi_k)$, and let w_k^ε solve

$$\begin{aligned} -\nabla \cdot (a_k^\varepsilon(x) \nabla w_k) - \lambda_0 \chi_k &= 0 & \text{in } B \setminus \bar{D} \\ \partial_{\nu_B} w_k &= 0 & \text{at } \partial B \\ \partial_{\nu_D} w_k &= f & \text{at } \partial D. \end{aligned} \quad (4.27)$$

(We assume here that χ_k satisfies the consistency condition for existence of w_k .) As $\varepsilon \rightarrow 0$, $\lim_{\varepsilon \rightarrow 0} w_k^\varepsilon$ minimizes

$$\int_{B \setminus \bar{D}} \chi_k(x) \left(\frac{1}{2} |\nabla w|^2 - \lambda_0 w \right) dx + \int_{\partial D} f w d\mathcal{H}^1,$$

in other words that it achieves the minimization over w in (4.12) (the proof parallels that of Lemma 3.1.5 in [1]). The advantage of introducing $\varepsilon > 0$ is that $a_k^\varepsilon(x)$ represents a mixture of two *nondegenerate* materials. Our understanding of structural optimization is rather complete in this setting: after passing to a subsequence, the possible *homogenization limits* $a_{\text{eff}}^\varepsilon$ of a_k^ε and the possible *weak limits* θ of χ_k are precisely those for which $a_{\text{eff}}^\varepsilon(x)$ lies in the G -closure of 1 and ε with volume fractions $\theta(x)$ and $1 - \theta(x)$ respectively (see e.g. Theorem 3.2.1 in [1]). The best microstructure is the one that maximizes the energy quadratic form $\langle a_{\text{eff}}^\varepsilon \nabla w, \nabla w \rangle$ at given volume fraction. This maximum is achieved by a layered microstructure, using layers parallel to the level lines of w , which achieves the well-known *arithmetic-mean bound*

$$\langle a_{\text{eff}}^\varepsilon \nabla w, \nabla w \rangle \leq (\theta + \varepsilon(1 - \theta)) |\nabla w|^2. \quad (4.28)$$

In summary: for the positive-epsilon analogue of our optimal design problem, the theory of homogenization provides a relaxed problem whose minimizers are precisely the weak limits of the minimizers of the original problem. It is obtained by replacing the term $\chi(x)|\nabla w|^2$ by the right hand side of (4.28) and the term $\chi(x)w$ by $\theta(x)w$. In the limit $\varepsilon \rightarrow 0$, this procedure gives exactly our relaxed problem.

The estimates justifying the results just summarized are not uniform as $\varepsilon \rightarrow 0$. As a result, the preceding argument cannot be used when $\varepsilon = 0$. In particular, it does not constitute a proof that our relaxed design problem is equivalent to the original one.

There is a related setting where an analogous relaxation has been justified even for $\varepsilon = 0$. The argument goes back to [12] and it can also be found in Section 4.2 of [1]. To briefly explain the idea, let us consider the optimal design problem

$$\sup_{\Omega \text{ s.t. } \overline{D} \subset \Omega \subset B} \inf_{w \in H^1(\Omega \setminus \overline{D})} \int_{\Omega \setminus \overline{D}} \left(\frac{1}{2} |\nabla w|^2 - \gamma \right) dx + \int_{\partial D} g w d\mathcal{H}^1, \quad (4.29)$$

where $\gamma > 0$ is a constant and g is a function on ∂D satisfying $\int_{\partial D} g d\mathcal{H}^1 = 0$ (so that the min over w is bounded below). This problem is very similar to (4.11), but the optimal w_* is now harmonic:

$$\begin{aligned} \Delta w_* &= 0 && \text{in } \Omega \setminus \overline{D} \\ \partial_{\nu_\Omega} w_* &= 0 && \text{at } \partial\Omega \\ \partial_{\nu_D} w_* &= g && \text{at } \partial D. \end{aligned} \quad (4.30)$$

Since (4.29) can be written as

$$\sup_{\Omega \text{ s.t. } \overline{D} \subset \Omega \subset B} - \int_{\Omega \setminus \overline{D}} \left(\frac{1}{2} |\nabla w_*|^2 + \gamma \right) dx,$$

it seeks the domain that minimizes $\int_{\Omega} \left(\frac{1}{2} |\nabla w_*|^2 + \gamma \right) dx$. Section 4B of [12] explains how this problem can be approached variationally. Briefly: extending $\sigma = \nabla w_*$ by zero to the entire set B , letting σ determine $\Omega = \{x : \sigma(x) \neq 0\}$, and using the principle of

minimum complementary energy as an alternative representation of $\int_{\Omega} \frac{1}{2} |\nabla w_*|^2$, one finds that (4.29) is equivalent to the minimization

$$\inf_{\substack{\operatorname{div} \sigma = 0 \text{ on } B \setminus \overline{D} \\ \sigma \cdot \nu_D = g \text{ at } \partial D \\ \sigma \cdot \nu_B = 0 \text{ at } \partial B}} \int_{B \setminus \overline{D}} \Phi_{\gamma}(\sigma) \, dx$$

with

$$\Phi_{\gamma}(\sigma) = \begin{cases} \frac{1}{2} |\sigma|^2 + \gamma & \text{if } \sigma \neq 0 \\ 0 & \text{if } \sigma = 0. \end{cases}$$

The relaxation of this problem is obtained by *convexifying* Φ_{γ} . A homogenization-based argument similar to the one presented earlier suggests (see [12]) that the relaxation should be obtained by replacing Φ_{γ} with

$$\min_{0 \leq \theta \leq 1} \frac{|\sigma|^2}{2\theta} + \gamma\theta. \quad (4.31)$$

This conclusion is correct, since (as verified in [12]) (4.31) is equal to the convexification of Φ_{γ} .

Can our relaxation of (4.11) be justified using an argument analogous to the one just summarized for (4.29)? Perhaps, however it seems that such an argument would require substantial new ideas.

Remark 4.7. *If, as we conjecture, the relaxation considered in Section 4.2 is equivalent to considering “homogenized” designs, then the saddle point provided by Theorem 4.3 would have $0 < \bar{\theta} < 1$ in any region where homogenization occurs. Reviewing the proof of that Theorem, we see that \bar{w} would need to have $\frac{1}{2} |\nabla \bar{w}|^2 - \lambda_0 \bar{w} = 0$ in such a region.*

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Declarations

Data availability is not applicable to this article, since no datasets were generated by this work.

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