Understanding New Regimes for Light-Matter Interactions

by

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B.S., University of California, Berkeley (2004)
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Submitted to the Department of Electrical Engineering and Computer Science
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Abstract

This thesis focuses on achieving new understanding of the principles and phenomena involved in the interaction of light with a variety of complicated material systems, including biomaterials and nanostructured materials. We will show that bone piezoelectricity may be a source of intense blast-induced electric fields in the brain, with magnitudes and timescales comparable to fields with known neurological effects, and may play a role in blast-induced traumatic brain injury. We will also shed new light on the localization of photons in a variety of complex microstructured waveguides. We will reveal the principles behind the design of single-polarization waveguides, including design strategies that did not seem to have been considered previously. Finally, we designed a 3D photonic crystal slab structure to exhibit negative-index behavior at visible wavelengths, which was fabricated and experimentally demonstrated by our collaborators to show negative refraction with, to our knowledge, the lowest loss at visible wavelengths to date.

Thesis Supervisor: Steven G. Johnson
Title: Associate Professor of Applied Mathematics
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This thesis is dedicated to You.
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Bovine and cranial specimens were tested with the Split Hopkinson bar. Copper leads were attached to the radial surface of the specimen $180^\circ$ apart.

Split Hopkinson bar results: Bovine specimens exhibited stress and polarization pulses of approximately the same time scale. Voltage response is correct order of magnitude: $V = \frac{d_{13}}{\epsilon_0 K} t \sigma_{33} \approx 40$ mV.

Schematics of various types of dielectric waveguides in which our theorem is applicable. Light propagates in the $z$ direction (along which the structure is either uniform or periodic) and is confined in the $xy$ direction by a higher-index core compared to the surrounding (homogeneous or periodic) cladding.

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A finite-difference time domain (FDTD) simulation confirms supercollimation behavior in our structure. Nitride thickness =245 nm, period=233 nm and radius= 78nm. A monochromatic point source with even parity, operating at the flat region of the first even band, is used. We observe a nice collimated beam on the other side. This is a cross section of the center of the nitride slab along the $z$ direction. The x-dimension of the diagram shown is about 10 μm, so the collimated beam has a transverse extent of about 1 μm.

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Gaussian beams approximating plane waves with incident angles of 4 and 7 degrees come in from the side of the structure with a nitride height of 78 nm, period of 260 nm, hole radius of 65 nm (top view).
This structure has a nitride height of 78 nm, period of 260 nm, with 200 nm of oxide on top and 200 nm of oxide below the nitride. The bottom layer sits on a silicon substrate. We show below the top view of the field pattern of the output field, i.e., just above the structure, assuming incident comes from the bottom of the figure. The \( y = 0 \) position is the point just emerged from the photonic crystal slab. We observe interesting spot patterns that appear periodically in the \( y \) direction. This is possibly due to the asymmetry in the actual structure, since we did not observe this when we used an infinite oxide layers above and below in our simulation. We can observe multiple intensity maxima (images) along \( y \). The image at 0.6 \( \mu m \) from the slab is not degraded by much from the one at 0.25 \( \mu m \), close to the slab, and even the third image at 1 \( \mu m \) is still quite distinguishable. The image distance of the third image is around the same as the object distance (around 1 \( \mu m \)).
This is the same structure as in Fig. 5-8 except that the heights of the top and bottom oxide layers are now decreased from 200 nm to 111 nm. Here, the stray spots on the side of the first main image along x=0 seem to overtake the image. The image at 0.65 μm is still distinguishable, albeit more weakly. However, the image at 1 μm has disappeared into the background noise. The degradation of performance can be explained as follows: Electric fields tend to concentrate in higher dielectric regions. Now that the bottom oxide thickness has been reduced, and recall that with our thin nitride thickness (set by various fabrication constraints), the photonic modes in this structure have fields that are not well localized in the nitride layer, or even the oxide layers, since the constraints are such that the total etch thickness can only be up to 300 nm. Thus, we get a lot of fields extending outside of the oxide-nitride-oxide sandwich, and the field profile will be skewed toward the silicon substrate instead of toward the air, lowering the frequency of the guided modes from the case with thicker oxide layers on top and below. We are therefore operating at a frequency above the flat band, since the flat band frequency of the structure has shifted down.

Fabricated structures.

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Chapter 1

Introduction

And God said

\[ \nabla \cdot \mathbf{D} = \rho \]

\[ \nabla \cdot \mathbf{B} = 0 \]

\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \] \hspace{1cm} (1.1)

\[ \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \]

And there was light.

— T shirts from the MIT COOP

The four partial differential equations known as Maxwell’s equations form the foundation of classical electrodynamics, classical optics, and circuit theory. They answer questions such as: Why is it that current flows in a loop of wire when the magnetic flux inside changes with time? Why is the sky blue? How are rainbows formed? We owe the great body of scientific knowledge about light and matter to scientists who were fascinated with questions such as these. The beauty and wonder of light continue to captivate scientists, and the study of light has marked the frontiers of physics with phenomena from the ultraviolet catastrophe to the photoelectric effect.

The discovery of the principles of electromagnetic theory and the use of such knowledge has transformed human life in a way unimaginable to our ancestors. The quest to understand electromagnetic phenomena and the interaction of light and mat-
ter has inspired countless innovative applications that have enabled human societies to move from agricultural to industrial; our generation can obtain the latest news and information at their fingertips using computers that have been connected to the Internet via high-speed glassy optical fibers.

Maxwell’s equations are elegant and accurate in regimes where light is “classical”, that is, when light can be considered a wave. However, their consequences in certain systems may be far from obvious: in structures with complicated geometries, one would need to numerically compute the solutions to even begin to understand the phenomena that are taking place. In other cases, one can prove theorems and make generalizations that add to our intuition. Still in more situations, the interactions are so complex that our focus is to design and take advantage of certain effects, rather than to fully comprehend these interactions.

This PhD thesis covers a variety of topics that are all connected to the interaction of light and matter with geometries that vary on the scale of the wavelength. The research included encompasses all the different cases alluded to above: from purely analytical derivations of mathematical conditions for waveguiding (confinement of light along a “wire”) in new classes of optical fiber, to the design of a flat lens, to the implementation of a 3D finite-element solver involving tens of millions of elements modeling what happens in the brain when a blast wave impacts the head. It ranges from basic scientific investigation in the case of the brain project to the design and engineering of a new device.

1.1 How shock waves can electrify your brain

There is an increasing use of improvised explosive devices (IEDs) in terrorist and insurgent activities. Exposure to blast waves is becoming more frequent, as reviewed in Ref. 186. Recent studies at certain military and marine units in Iraq reveal that close to 90 percent of military personnel injuries were by explosions, mostly by IEDs. About 50 percent of these involved the head or neck. Many soldiers suffer from traumatic brain injuries (TBI). Patients with mild TBI often experience memory loss,
sleep disturbances, headaches, confusion, dizziness, blurred vision and sensitivity to light and noise [163,186,200]. Those with moderate or severe TBI may also show these symptoms, as well as vomiting, nausea, loss of coordination, weakness or numbness of the extremities, convulsions and seizures [163,186,200]. The more conventional cases of traumatic brain injuries (TBI) involving shrapnel impacting the head (known as ballistic trauma) are easily identified and diagnosed. However, there are many cases in which soldiers were rendered dazed or unconscious by an explosion that caused no externally visible injury [120].

Historically, many cases associated with these symptoms were diagnosed as a mental/psychological problem known as post-traumatic stress disorder (PTSD), a term coined during WWI [191]. However, recent statistics point to a possible physical source of these symptoms beyond merely psychological effects. In particular, of the first 433 patients diagnosed with TBI at the Walter Reed Army Medical Center between January 2003 and April 2005, data indicated that 88 percent were closed-head TBIs and 68 percent were blast related [120]. These point to the possibility that the shockwave itself can be a source contributing to TBI as it passes through the head. This is the subject of ongoing research at MIT and elsewhere [26,127,129,186], although relatively little is known about the exact physical mechanism by which the shockwave affects the brain.

Because so little is currently known about this problem, we chose to complement other groups’ investigations of purely mechanical effects by looking at something different. We studied a potential source of TBI that had not been previously considered [26] and, at first, may appear completely unrelated to mechanical shock waves: electromagnetic pulses (EMPs) [49,93]. Very little is known about the electromagnetic fields that are induced in the brain by an IED-scale explosion, and at first glance the most obvious source of such fields is the EMP produced by the detonation process itself [49,54,71]. However, this EMP turns out to be strongly damped by the dielectric properties of the brain—which mostly counteracts any external EMP by polarization—while we discovered that a potentially much larger source of EMP actually stems from the shockwave itself as it impacts the head [106]. In particular,
we noticed that researchers in an unrelated context had reported bone to be a piezoelectric material: bone electrically polarizes under stress [7,24,57,204]. This means that, when a blast wave impacts the head and creates a pulse of large stresses in the skull, a corresponding EMP may be generated directly in the brain adjacent to the skull. There is actually quite a bit of medical information on the magnitude of electric fields that are needed to affect neurological processes [3,83,196], so by computing these piezoelectric fields we were able to theoretically establish at least the possibility that this EMP may actually play a role in TBI [106].

This piezoelectric EMP phenomenon is schematically depicted in Fig. 1-1. First, an incoming blast wave in the air impacts the soldier's head, a process that has been modeled in great detail by mechanical simulations of our colleagues [127]. Stresses are induced in the tissues in the head, and we calculate the resulting electrical polarization created via the bone piezoelectric effect, which in turn yields an induced charge density. The presence of these charge densities produce an electric field. We solve for these fields computationally using a finite element model of the head—a large numerical problem involving millions of elements describing the fields in every tissue region—and find that the order of magnitude of these electric fields to be as high as 20 V/m, which agrees with and slightly exceeds the simple estimate from assuming that the charge density is uniform sheet. Volumes on the order of $10^5 \text{ mm}^3$ of the brain are exposed to fields $|\mathbf{E}| > 0.3 \text{ V/m}$, the IEEE safety standard for the general
public [83], and volumes on the order of $10^4$ mm$^3$ exceed the 0.9 V/m standard for controlled environments. Brain volumes of a few mm$^3$ are exposed to $|E| > 9$ V/m, which exceeds the IEEE threshold by an order of magnitude and reaches values comparable to repetitive transcranial magnetic stimulation (rTMS) [131, 195, 196], a medical procedure that intentionally disrupts brain functions and induces longer-term effects by stimulating the release of neurochemicals.

Our predictions are currently stimulating efforts to measure piezo-induced EMPs in bone, and in particular to measure piezoelectric properties of human cranial bone (whereas all previous measurements were mainly for human and animal tibiae and femurs).

1.2 Mathematical conditions for your browser to access websites in Japan

A waveguide is a structure that directs where waves, such as electromagnetic waves, travel. They come in different shapes, sizes, and materials, and confine waves in certain directions but “guide” them in the propagation direction(s). They could be anything from metallic co-axial cables that guide microwave and lower frequencies [96], to conventional silica-glass optical fibers guiding light of infrared or visible frequencies [180]. Typically, a waveguide confines light within a “core”, surrounded by a “cladding” that is responsible somehow for the confinement. At microwave frequencies, metal is a good mirror and the cladding can simply be a metallic tube confining waves within an air core [96]. At infrared frequencies, metals have much higher absorption losses, so most optical fibers instead use “total internal reflection”: a core with a higher index of refraction is surrounded by a cladding with a lower index of refraction [180]. Recently, more exotic waveguides known as photonic crystal fibers or microstructured optical fibers, have been developed [87, 88, 128].

For example, by putting periodic microstructures—such as an array of air channels—in an otherwise transparent glass cladding, one can create a “photonic bandgap” that
makes the cladding a perfect reflector at certain wavelengths and incident angles [87].
This allows one to achieve unusual waveguiding effects such as guiding light within a
hollow (lower index) air core [50,88,88,128,140]. Hollow-core fibers reduce the interaction
of light and the core, thus reducing absorption and allowing broader bandwidths
and access to wavelength regimes that are hard to explore with solid-core fibers.
One can therefore efficiently introduce small volumes of gases into the hollow core
for chemical sensing in applications such as pollution monitoring or national security [25,88,128,159,179]. Hollow fibers are also used in medical applications, where
they act as a flexible medium in endoscopy to transmit power from CO₂ lasers to a
target within the human body for ablations in surgery [128,188]. Previous fibers were
unable to perform this role as the CO₂ laser power would heat the material in the
solid core so much that it would melt [188].

Instead of a hollow core, one can use a solid glass core but surround it with a
cladding that is again perforated by air holes (as shown in Fig. 1-2[b]), forming “on
average” a much lower index of refraction than the core. This permits very strong
confinement, for example to enhance nonlinear optical effects. Optical nonlinearities
can be exploited to obtain a number of useful phenomena: optical solitons [48,69,
177,194], which are pulses that don’t spread out as they propagate; conversion of
light at one wavelength to another wavelength [4,27,78,132]; generation of white
light (many colors) from a single input wavelength (an effect called supercontinuum
generation) [33,40,103,110].

Understanding the confinement and guidance mechanisms of the various types
of waveguides is crucial because of their indispensable role in so many applications.
However, there are only a handful of geometries for which analytical solutions are pos-
sible. Even in such cases, the solutions are often hard to understand. For example,
in step-index fibers, the solutions are solutions of transcendental equations involving
Bessel functions [180]. It is particularly hard to study guidance in microstructured
fibers analytically, although brute-force computational solutions are certainly possible [89].

We look at waveguides in Chapter 4, and in particular these new classes of mi-
crostructured dielectric waveguides, at a more fundamental level, to gain a more
general understanding of confinement and guidance. We establish and prove a suf-
ficient mathematical condition for the existence of index-guided “modes” [180], or
what we can think of as channels in which signals can propagate, in a very general
class of dielectric waveguides, including photonic-crystal fibers (with arbitrary peri-
odic claddings, such as “holey fibers”), anisotropic materials, and waveguides with
periodicity along the propagation direction, as illustrated in Fig. 1-2 [109]. Our con-
dition provides a rigorous guarantee that a mode can exist for any frequency as long
as we have a waveguide core with “on average” a high dielectric permittivity, where
electric fields tend to concentrate (to be described more later).

On a basic level, our theorem is similar to what happens in the special case of a
traditional step-index fiber, where light is confined in the core with raised dielectric
in the 2D plane, and propagates down the third direction. The mechanism, known
as index-guiding, is analogous to the simplistic picture of “total internal reflection”,
where light rays at certain angles become totally internally reflected at the interface
with a lower dielectric [167]. This analogy is plausible in the case of a “holey fiber”,
for example, because the dielectric cladding with air holes has a lower “average”
index than the filled dielectric core [87]. Since our result is intuitively plausible, it
may appear to some that it is “obvious”. However, it should be born in mind that
the history of mathematics is littered with the bodies of mathematicians who have
tried and failed to prove the obvious, and in some famous cases people attempted
for thousands of years to prove “obvious” facts that turned out to be false (e.g.
squaring the circle [20]). Even in the case when intuition prevails, as it does for
our case, such proofs add to the foundation of mathematics. In fact, there exist a
number of subtleties here. First, an intuitive expectation of a guided mode for non-
traditional structures such as photonic crystal fibers, is far from a rigorous guarantee.
Even when the core is formed by strictly increasing the dielectric, researchers had
suspected that there might not be a guided mode at every wavelength, but rather
that the fundamental (lowest-frequency) mode may be a long-wavelength cutoff (as
was initially suggested in holey fibers [102], but was later contradicted by more careful
[a] Cross section of a waveguide (e.g. a conventional fiber) with a homogeneous cladding and an arbitrary-shape core.

[b] Cross section of a photonic-crystal fiber with periodic cladding and arbitrary-shape core.

[c] A waveguide periodic in the propagation (z) direction surrounded by a homogeneous cladding.

Figure 1-2: Schematics of various types of dielectric waveguides in which our theorem is applicable. Light propagates in the z direction (along which the structure is either uniform or periodic) and is confined in the xy direction by a higher-index core compared to the surrounding (homogeneous or periodic) cladding.

Therefore, our theorem is valuable in providing an absolute guarantee, with no calculation required, that strictly increasing the refractive index to form the waveguide (e.g. filling in a hole of a holey fiber) yields a guided mode for all frequencies, known as a cutoff-free guided mode. Furthermore, our theorem highlights the parallels between electromagnetism and other wave phenomena, because our proof is closely related to the proof of a famous theorem from quantum mechanics, in which any attractive potential in two dimensions was shown in 1989 to localize a quantum wave [205].

numerical calculations [203]). Second, when the fiber core consists of partly increased and partly decreased dielectric index, precisely how much decreased-index regions does one need to have such a cutoff?
1.2.1 The development and design of single-polarization single-mode/SPSM fibers

In a conventional fiber, there are two “polarization modes”, or “polarizations”, which we can think of as channels, for waves to propagate with different orientations [180]. (The electric field is a vector whose magnitude and direction can vary with time, and in a wave the direction of the field is mostly perpendicular, or “transverse,” to the direction of propagation.) In a conventional optical fiber with a circular core, the symmetry means that both polarizations travel at the same speed (they are “degenerate”). Because of this, the fiber can still be thought of as having a single propagation channel, and it is termed “single mode” even though there are really two modes [153]. However, the existence of two polarization solutions leads to two major complications.

First, after light propagates down a long fiber, the polarization coming out at the end of the fiber is essentially random. This greatly complicates the design of optical devices to work with fiber inputs, since many integrated devices tend to be polarization sensitive [153]. (In fact, the polarization at the end of the fiber will even change over time, as small variations such as temperature changes—which slightly change the refractive index—will result in a different polarization at the end facet.)

Second, real fibers are not exactly circularly symmetrical, and so the two polarizations do not travel at exactly the same speed. There are many sources of imperfection that can break the symmetry: manufacturing imperfections, bending of the fiber, stresses, and so on [180]. This means that an arbitrary input polarization is decomposed in the fiber into two polarizations that travel at slightly different speeds, causing signals to spread and distort as they pass through the fiber. This effect is called “polarization mode dispersion” (PMD) [153], and is difficult to correct because it results from a random (even time-varying) process. Ultimately, one can only compensate for such distortions by sending data at a lower rate through the fiber: data consists of pulses representing “bits” of information, and if the pulses are far enough apart (i.e. a slow enough bit rate) then they can spread without interfering.

One solution to both of these problems is to use a polarization maintaining fiber
A PMF supports two polarization modes, but the symmetry is intentionally broken by so much that the polarizations travel at very different speeds—for example, by using an elliptical core [134]. This means that, if you launch light with one polarization into a PMF, it will tend to stay in that polarization. However, a big enough imperfection can still cause light in a PMF to scatter from one polarization to the other, so there is still some “crosstalk” and interference.

An ideal way to prevent crosstalk is to have a fiber that supports propagation in just one polarization, removing the possibility for the signal to cross-couple and interfere with the other polarization altogether. Such fibers are known as \textit{single-polarization single-mode} (SPSM) waveguides: waveguides that are \textit{truly single-mode} in the sense of supporting only a single guided-mode solution. Many designs of SPSM fibers have been proposed [29-31, 42, 43, 47, 51, 91, 94, 99, 111, 112, 114, 115, 123, 137, 138, 161, 165, 175, 181, 183, 185, 187, 208, 212]. However, prior to our work, there did not seem to be any systematic studies of the conditions for obtaining a SPSM bandwidth in a fiber. Such rigorous conditions would be very desirable for both mathematical interest and for guiding practical designs. In fact, it turns out to be provably impossible to have just one polarization but not the other in most types of conventional fibers. We show the necessary conditions for SPSM operation by extending our previous work on the existence of guided modes in microstructured dielectric waveguides to derive conditions for having \textit{two} guided modes, and identify different strategies for achieving SPSM fibers. At least one of the strategies that we identify represents a new type of SPSM fiber that was not previously considered, illustrating the benefit of having a rigorous theory [108].

1.2.2 Bandgap guidance in the Schrödinger operator

The emergence of new types of optical fibers have opened up new possibilities of wave guidance by mechanisms other than index-guiding. One commonly employed guidance mechanism is photonic bandgap guidance [87, 100]. Physically, bandgaps are frequency windows over which there can be no extended light modes in the structure. Incident light within the bandgap of a photonic crystal structure gets completely
reflected. Waveguides based on this principle have been designed and employed in fields from astrophysics to medicine [77, 128, 188]. Because of the widespread usage and importance of these waveguides, we would like to have an analogous condition on the existence of bandgap-guided modes.

We mentioned above that our proof of index guiding in microstructured fibers was related to a similar proof in quantum mechanics (where the mathematics is actually much simpler because the wave equation there is simpler, e.g. quantum waves are scalars rather than vectors) [205]. So, when considering bandgap guidance in optical fibers it is natural to start with the analogous quantum result: confinement in crystals with electronic bandgaps using defects in the crystal. However, there was no such result — no one had proved the requisite confinement conditions in more than one dimension even for quantum mechanics. Both as a prerequisite for the electromagnetic case, and because quantum confinement by bandgaps is of fundamental interest in its own right for solid-state physics [8], we therefore set out to prove conditions for quantum bandgap confinement. Although I suggested a general strategy for such a proof in my index-guiding paper [109]—the basic idea involves squaring a certain operator (adapting a technique by Kuchment and Ong [100]—the execution of this approach was carried out by a very talented summer student, Arthur Parzygnat, whom I helped to supervise. The resulting proof [141] is included at the end of Chapter 4.

1.3 Design of flat lens at visible wavelengths

A lens is a transparent optical device which transmits and refracts light such that the outgoing beam gets focused or spread out (converged or diverged). If you are farsighted, for example, your spectacles will usually consist of two convex lenses, as shown in Fig. 1-3[a]. You may recall Snell’s law from high school, in which the incident angle $\theta_i$ is related to the refraction angle $\theta_r$ by the indices of refraction $n_i$ and $n_r$ of the two materials: $n_r \sin \theta_r = n_i \sin \theta_i$ [167]. With such conventional lenses, a curved surface is necessary to bend the rays in the desired directions, and focused spots can
only be made from objects that are sufficiently far away (which is why your cheap camera can't focus on a fly walking on the camera lens).

All natural transparent materials, such as glass, exhibit positive indices of refraction, in which case incident rays are refracted “forwards” to rays on the opposite side of the surface normal, as in Fig. 1-4[a]. Russian physicist Veselago proposed the theoretical possibility of materials with negative indices of refraction in 1968 [193], which would cause the rays to refract “backwards”, onto the same side of the normal, as in Fig. 1-4[b]. This permits a fundamentally different type of imaging, as shown in Fig. 1-3[b]: imaging of an nearby object by a flat lens. More recently, Pendry [142] suggested that negative refraction can theoretically lift the fundamental diffraction limit of conventional lenses, to make a “perfect lens” or “superlens”. Although Veselago’s proposal was purely theoretical—he did not know how to make such materials—more recently Pendry and others have proposed “metamaterials” that achieve an effective negative index by using subwavelength microstructure [143,144,169,182]. These subwavelength (typically metallic) structures become increasingly difficult to fabricate and, worse, increasingly absorptive [39,169,210], at short wavelengths (infrared and visible)—for example, a recent low-loss metallic metamaterial structure still has an absorption length of only a few microns [206]. Instead, an alternative approach is to mimic negative refraction and superlensing phenomena with wavelength-scale (not subwavelength) microstructures, in which the propagation of light is more complicated than a simplistic ray picture can capture [116–118,135]. Such “negative-index behaviors” (NIBs) via wavelength-scale structures in transparent materials is the approach that we explore in this thesis, in which our goal was to push negative refractive phenomena down to visible wavelengths (motivated by lithography applications) without incurring large absorption losses.

The resolution of conventional lenses is limited by the Abbe-Rayleigh diffraction limit, which results from the loss of high spatial-frequency wavevector components, corresponding to evanescent waves that become exponentially small in the far field [52]. For a long time, it was believe that subwavelength features of objects could not be imaged. Since Pendry’s proposal of the “perfect lens” [142] in 2000, there has
been much excitement about the prospect of negative-index behavior (NIB) such as superlensing in a flat lens and supercollimation, which conventional lenses are incapable of producing. The key point is that, because a flat lens can image nearby objects (objects in the “near field”), the evanescent waves have not entirely disappeared and it is possible to resonantly amplify them to reconstruct a subwavelength image [142,211]. In Pendry’s case, this resonant amplification is automatically achieved if the requisite negative index of refraction is present, but such negative indices are very difficult to achieve at short wavelengths without incurring large absorption [39,169,206,210,211]. Alternatively, in flat lenses made from wavelength-scale structures, similar resonant transmission of evanescent waves can be achieved by careful design of “surface states” at interfaces [117]. Imaging beyond the diffraction limit could allow for a new class of industrial nanolithography and make possible entirely new kinds of nanomaterials [17], while flat lenses (Fig. 1-3[b]) could be used on everything from displays to sensors. In order to be feasible for such applications, however, one must be able to work with short (visible) wavelengths—it does no good to image at 1/10 of the wavelength resolution if your wavelength is 10 times larger than that of state-of-the-art conventional lithography [17], for example.

Before one attempts to attain subwavelength imaging by capturing evanescent waves, however, a first step is to attain the negative refraction NIB, which by itself is potentially useful for flat-lens imaging even if the resulting image is not subwavelength. Such imaging, as mentioned above, has the unique property of imaging objects in the near field, not limited by the focal length of a traditional lens, and so may have various applications for integrated devices. Even achieving negative refraction alone, however, turns out to be very challenging at visible wavelengths if one wishes to also obtain low loss, since transparent materials at visible wavelengths tend to have relatively low index contrast (a problem for devices based on strong diffraction phenomena). We are not aware of any previous experimental work that has achieved similarly low-loss negative refraction at visible wavelengths (the best competing structure [206] has absorption an order of magnitude worse).

We designed a 3D photonic crystal slab device to exhibit negative refraction at
visible wavelengths, using physical principles similar to those described by Luo et al. in 2D and 3D crystals (but using much larger refractive indices than are available to us) [116, 118]. The challenge here is the limitations in material choices — a larger dielectric index contrast helps, but as wavelength decreases, the attainable contrast decreases. Our goal is to realize negative refraction and flat-lens imaging in visible wavelengths for use as a basic starting point for progress in applications of this technology such as those mentioned above. Based on our theoretical designs, our experimental collaborators fabricated the structure and obtained measurements in qualitative agreement with the theory.
[a] A convex lens focuses rays that are initially diverging. The curvature is crucial for naturally occurring transparent dielectrics.

[b] Negative-index behavior (NIB) materials can be used to form a flat lens that focuses light from an object in the near field.

Figure 1-3: Lenses made of a natural material and a negative-index behavior material
[a] A light ray incident on the interface of a natural transparent material bends “forwards” to rays on the opposite side of the surface normal.

Figure 1-4: Positive and negative refraction

[b] A light ray incident on the interface of a NIB material bends “backwards” onto the same side of the surface normal.
Chapter 2

Some Background on Maxwell’s equations, Photonic Crystals, and Bandgaps

2.1 Maxwell’s equations and matter

As alluded to in the last chapter, Maxwell’s equations are the foundation of classical electrodynamics and classical optics. We shall now take a closer look at them:

\[
\begin{align*}
\nabla \cdot \mathbf{D} &= \rho \\
\nabla \cdot \mathbf{B} &= 0 \\
\n\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\
\n\nabla \times \mathbf{H} &= \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}
\end{align*}
\]  

(2.1)

Here, \( \mathbf{E} \) and \( \mathbf{H} \) are the macroscopic electric and magnetic fields, \( \mathbf{D} \) and \( \mathbf{B} \) are the displacement and magnetic induction fields, and \( \rho \) and \( \mathbf{J} \) are the free charge and current densities [86]. In a region of linear, mixed dielectric medium, the fields are furthermore related as follows:
\[
D_i = \epsilon_0 \sum_j \epsilon_{ij} E_j + \sum_{j,k} E_j E_k + O(E^3) \tag{2.2}
\]

\[
B = \mu_0 \mu H
\]

where \( \epsilon_0 \approx 8.854 \cdot 10^{-12} \) Farad/m is the permittivity of free space. In this thesis, we are concerned with nonmagnetic materials, and we therefore set \( \mu \) to 1. For our purposes, the field strengths are small enough for us to approximate the nonlinear terms to zero.

Physically, the dielectric permittivity tensor describes the effective screening of electric field in a given material. In particular, the displacement field is given by:

\[
D = \epsilon_0 E + P = \epsilon_0 (1 + \chi) E \tag{2.3}
\]

where \( P \) is the electric polarization, which is the dipole moment per unit volume. When an electric field is applied to a dielectric material, the molecules inside the material tend to rotate and redistribute (or, “polarize”) in order to partially cancel the electric field, thus “screening” the field [86]. This screening effect turns out to be quite important for the blast-induced fields in the brain, as we shall see in Chapter 3.

2.2 Eigenmodes and eigenfrequencies of light modes

In general, electric and magnetic fields are functions of time and space. Because Maxwell’s equations are linear, we can expand the time-dependent fields in a set of harmonic modes [86]:

\[
E(r, t) = E(r, \omega)e^{-i\omega t} \tag{2.4}
\]

\[
H(r, t) = H(r, \omega)e^{-i\omega t}
\]

For the sourceless (no free charge \( \rho \) and free current \( J \)) case, we can substituting the above expansion into the two curl equations in eq. (2.1), and obtain, for each
frequency \( \omega \):

\[
\nabla \times \mathbf{E}(r) - i\omega \mu_0 \mu \mathbf{H}(r) = 0
\]

\[
\nabla \times \mathbf{H}(r) + i\omega \varepsilon_0 \varepsilon(r) \mathbf{H}(r) = 0
\]

Eliminating \( \mathbf{E} \) above, we have derived the master equation:

\[
\nabla \times \varepsilon(r)^{-1} \nabla \times \mathbf{H}(r) = \frac{\omega^2}{c^2} \mathbf{H}(r)
\]

where \( c = 1/\sqrt{\varepsilon_0 \mu_0} \) is the vacuum speed of light [87]. Equation (2.6) is in fact an eigenvalue problem: \( \mathbf{H}(r) \) is the "eigenfunction" or "eigenmode", the multiplicative constant \( \omega^2/c^2 \) is the "eigenvalue", and \( \omega \) is known as the "eigenfrequency". For a given structure \( \varepsilon(r) \), we can obtain the spatial profiles of the magnetic field \( \mathbf{H}(r) \), as well as the corresponding resonant frequencies, for these eigenmodes. Physically, an eigenmode is a spatial profile of light at a given frequency that is excited and persists when incident light of this matching frequency is launched into a given structure. In a homogeneous medium, the eigenmodes are just plane waves traveling at the speed of light in the medium \( c/n \), where \( n = \sqrt{\varepsilon} \) is the dielectric index. However, in structures with dielectric modulations on the order of the wavelength, the behavior can be very different. In particular, we would like to focus on the basic theory of microstructured photonic crystals in the next section.

2.3 Bloch's Theorem and Photonic Crystals

Photonic crystals (PCs) are man-made materials with periodicity in 1D, 2D or 3D, designed to mold and control the flow of light [87]. In order to analyze the behavior of photonic crystals, it would be beneficial for one to understand what the symmetries of a dielectric structure can tell us about its electromagnetic eigenmodes. It turns out that we can write the magnetic field of a given mode in a photonic crystal as:

\[
\mathbf{H}_k(r) = u_k(r)e^{ikr}
\]

\[ \text{(2.7)} \]
where \( u_k(r) \) is a periodic function with the same periodicity as the photonic crystal itself, whatever the dimensionality of periodicity. This is known as “Bloch’s theorem”, a theorem that stems from solid state physics [8,87]. In a way, it is the generalization of the form \( H_0 e^{ikr} \) for plane wave solutions in a homogeneous medium. The relationship between the frequency and “k-vector”, or “propagation constant”, \( k \) (in directions of discrete or continuous translation symmetry, where \( k \) is well defined), is known as the photonic “dispersion relation” [87], analogous to their electronic counterpart in materials with periodic crystalline structures, such as silicon and germanium [8]. Here, the \( k \) vectors in the 2D plane are conserved, and \( \omega \) is a function of this set of wavevectors. We show the dispersion relation of a 2D photonic crystal structure made of a square array of cylindrical dielectric columns in Fig. 2-1. Such band diagrams are usually plotted around the irreducible Brillouin zone edge [87] (The Brillouin zone is the Wigner-Seitz cell in the wavevector \( k \)-space. [8]), as is the present case. There is a range of frequencies (shaded in yellow) for which no eigenmodes of the TM polarization exist. Such bandwidths are known as “photonic bandgaps” in analogy with electronic bandgaps in, for example, semiconductors, where no electronic states are available. Incident light with frequencies within bandgaps becomes completely reflected, since there are no available states for it to occupy within the PC [87]. PCs can therefore be employed as high quality mirrors for use in many exciting applications. For example, by introducing “defects” in the form of a line (e.g., in Fig. 2-2) or a cavity (e.g., in Fig. 2-3) that breaks the perfect periodic symmetry, light can be confined in these defects in devices such as novel waveguides and lasers [87]. Three-dimensional photonic crystal fibers, or microstructured fibers, operate based on similar principles by confining light in the transverse plane of the fiber cross section, but allowing propagation in the third direction [87]. Some examples are shown in Fig. 2-4. A detailed discussion on the “index-guiding” mechanism of the lowest-frequency guided modes for structures in Fig. 2-4[b] (and Fig. 2-4[c]) is provided in Chapter 4, and the quantum parallel of bandgap guidance in structure Fig. 2-4[b] is provided in Sec. 4.3. The Bragg fiber in Fig. 2-4[a] guides light by acting as an omnidirectional reflector under the light cone, which is distinct from the mechanisms
Figure 2-1: (Figure from Ref. 87.) The photonic band structure for a square array of dielectric columns with $r = 0.2a$. The blue bands represent TM modes and the red bands represent TE modes. The left inset shows the Brillouin zone, with the irreducible zone shaded light blue. The first TM photonic bandgap is shaded in yellow. The right inset shows a cross-sectional view of the dielectric function. The columns ($\varepsilon = 8.9$, as for alumina) are embedded in air ($\varepsilon = 1$).

that we consider in this thesis [87,88].

Sometimes, one is not merely interested in frequency extrema (which are likely to appear only on the boundary of the irreducible Brillouin zone and not in the interior, although there has yet to be a proof for this). Designing PC structures for negative refraction, for example, requires knowledge of frequency contours in the full 2D Brillouin zone. Chapter 5 details the principles for the phenomenon of negative refraction in a PC slab structure (2D periodicity in a structure of finite height), and the design of such a structure.
Figure 2-2: (Figure from Ref. 87.) Electric-field ($E_z$) pattern associated with a linear defect formed by removing a column of rods from an otherwise-perfect square lattice of rods in air. The resulting field, shown here for a wave vector $k_y = 0.3 \ (2\pi/a)$ along the defect, is a waveguide mode propagating along the defect. The rods are shown as dashed green outlines.

Figure 2-3: (Figure from Ref. 87.) Point-defect cavity formed by a single missing rod in a square lattice of radius 0.2a dielectric rods ($\varepsilon = 11.4$) in air. The cavity supports a single mode of frequency $\omega a / 2\pi c = 0.38$, inside the TM bandgap, whose electric field $E_z$ is shown.
Figure 2-4: *Figure from Ref. 87.* Three examples of photonic-crystal fibers (cross sections). [a] Bragg fiber, with a one-dimensionally periodic cladding of concentric layers. [b] Two-dimensionally periodic structure (a triangular lattice of air holes, or "holey fiber"), confining light in a hollow core by a bandgap. [c] Holey fiber that confines light in a solid core by index guiding.
In this chapter, we show that bone piezoelectricity—a phenomenon in which bone polarizes electrically in response to an applied mechanical stress and produces a short-range electric field—may be a source of intense blast-induced electric fields in the brain, with magnitudes and timescales comparable to fields with known neurological effects, and may play a role in blast-induced traumatic brain injury.

We compute the induced charge density in the skull from stress data on the skull from a finite-element full-head-model simulation of a typical IED-scale blast wave incident on an unhelmeted human head as well as a human head protected by a kevlar helmet, and estimate the resulting electric fields in the brain based on simple charged-sheet (1D) electrostatic approximations, finding electric fields on the order of 10 V/m in millisecond pulses [106]. Furthermore, we combine full-head-model blast-wave simulations with three-dimensional finite-element electrostatics solvers to compute the three-dimensional electric field produced in a human brain as a result of the skull’s piezoelectric response to the blast wave impacting the head, and find that the resulting in-brain fields are up to ~ 20 V/m for millisecond blast wave pulses. Field magnitudes of both our simple estimation and 3D simulations are more than one order of magnitude greater than IEEE safety standards [83] and comparable to those in medical procedures (transcranial magnetic stimulation, TMS) designed to
have neurological effects [131, 195, 196]. Moreover, brain volumes on the order of $10^5 \text{ mm}^3$ are found to be exposed to fields $|E| > 0.3 \text{ V/m}$, the IEEE safety threshold for the general public [83]. Similarly, brain volumes on the order of $10^4 \text{ mm}^3$ are found to be exposed to fields $|E| > 0.9 \text{ V/m}$, the IEEE safety threshold in controlled environments [83]. Brain volumes on the order of a few mm$^3$ are found to be exposed to fields as high as $9 \text{ V/m}$, which is 10 times the IEEE safety threshold in controlled environments. Such order-of-magnitude results indicate that more theoretical and experimental study of the subject is in order.

The remaining chapter is organized as follows. In Sec. 3.1, we first review some known mechanisms by which electromagnetic fields may be generated in explosions, and known safety levels of electromagnetic fields. We then summarize the available measured data of bone piezoelectricity in literature in Sec. 3.2. We introduce our computational model in Sec. 3.3, describing how we compute the blast-induced charge densities and electric fields in more detail in Sec. 3.3.1 and giving simple estimates of these in-brain electric fields in Sec. 3.3.2. Section 3.4 presents the results of our simulations. Sec. 3.5 describes our collaborators’ measurements of the piezoelectric coefficients of bovine femurs and porcine skull. Finally, we mention some future directions to pursue in Sec. 3.6.

### 3.1 Known safety levels and mechanisms for electromagnetic field generation in explosions

In order to assess the potential neurological impact of any blast-induced electromagnetic fields in the brain, we compare them to published safety standards and also to medical procedures where neurological effects are intentionally induced in the brain via electric fields. At millisecond timescales (ms pulses, $\approx 1 \text{ kHz}$ frequencies) typical of IED-scale blasts, the IEEE safety threshold for in-brain electric fields is $0.3 \text{ V/m}$ for the general public and $0.9 \text{ V/m}$ in controlled environments [83]. Another point of reference is the medical procedure rTMS, which uses magnetic-field pulses
to create electric fields in the brain that, in turn, induce currents which can disrupt brain activity in the short term or have longer-term effects by stimulating the release of neurochemicals [131,195]. A recent full-head finite-element simulation of a typical commercial rTMS device found maximum in-brain current densities of around 4.4 A/m² (in ms-scale pulses) [196]; the brain has a conductivity of about 0.28 A/Vm at kHz frequencies [196], and hence this generates in-brain electric fields of up to 4.4/0.28 ≈ 16 V/m. Even stronger long-term neurological effects, such as retrograde amnesia, are produced by electroconvulsive therapy (ECT), which uses ms current pulses repeated several times a second with amplitudes up to 1 A [3]; given the conductivity of the brain and the fact that the ECT current travels over a distance of around 20 cm, a simple dimensional analysis gives an estimated in-brain electric field of (1 A)/(0.28 A/Vm)/(0.2 m)² ≈ 100 V/m. All of these procedures utilize millisecond pulses because that is the timescale of the neuron action potential [13], and this unfortunately also means that the millisecond pulses induced by IED-scale explosions are on a timescale that is neurologically relevant.

An explosion can produce electromagnetic (EM) fields in several ways. First, the initial explosion generates a flash of EM radiation (including visible light), which is measurable far away [1,19,49,93]. In evaluating fields generated outside the brain, however, it is important to realize that such fields are reduced in the brain by a factor of roughly the relative permittivity of brain matter [86], which is about 10⁵ at the neurologically important kHz frequencies. [59] Although EM pulses from this initial flash continue to be studied in many contexts, here we instead consider the generation of EM fields from the supersonic blast wave itself (outside of the detonation region where the initial flash is generated). For example, the supersonic shock front is associated with a temperature increase that can ionize particles in the gas or other materials it passes through, but a simple estimate suggests that the resulting fields are orders of magnitude below the IEEE safety limits for IED-scale explosions in air (See Appendix 3A). Also, a high-pressure blast front can polarize water molecules (and other polarizable particles), an effect which has been observed to yield electric fields up to 200 V/m for very high pressures (100 kbar) corresponding to nuclear-scale
explosions, [2, 54, 67, 68, 70, 71, 113] but this effect should be negligible for IED-scale blasts where the pressures are much lower (0.02 kbar [127]). Finally, much larger EM fields can be generated when the high-pressure blast wave impacts a piezoelectric material [155, 172], which polarizes even in response to low pressures (and are therefore used as pressure sensors and actuators for a variety of applications [5, 36, 133, 172]). Here, the key fact is that bone is known to be a strongly piezoelectric material [7, 11, 16, 24, 32, 57, 66, 147, 158, 176, 204]: even though a polarized piezoelectric material is neutral (no net charge) and the resulting fields are short range, the adjacency of skull bone to the cerebral cortex means that even short-range fields may be relevant to TBI if they are strong enough.

3.2 Bone piezoelectric response

Piezoelectricity is the phenomenon in which an electric polarization is generated in response to an applied mechanical stress:

\[ P = d \sigma \]  

(3.1)

where \( P \), \( d \), and \( \sigma \) are the polarization density, piezoelectric tensor (a property of the material), and stress tensor, respectively [21]. It is well known that the piezoelectric effect occurs in certain classes of crystals and ceramics. Numerous efforts to measure such properties in biomaterials have been undertaken. In particular, Fukada and Yasuda demonstrated a piezoelectric response in dry bone at 2 kHz in 1957 and measured a typical piezoelectric coefficient, \( d_{14} \) (described below), to be 0.2 pC/N [57] (about one tenth of the value for quartz). Subsequent measurements have shown that piezoelectricity is also present in wet bone [11], live bone [16, 32], and in other biomaterials such as tendons [204], collagen [56], skin [170], and blood-vessel walls [55]. Reinish and Nowick established that moisture level plays a role in bone piezoelectricity [158], and Pfeiffer studied the effect of the frequency of the applied stress on bone piezoelectricity (i.e., material dispersion) [147]. Bur [24] studied bone piezoelectric
properties as a function of temperature and humidity in the range $10^{-2}-10^2$ Hz. An extensive summary of these measurements can be found in Ref. 176, and more recent measurements were described in Ref. 66 and Ref. 7. These values were all measured for animal or human tibiae and femurs, and the measured piezoelectric coefficients have some variability but remain within the same order of magnitude: the largest components of $d$ are all on the order of 0.1 pC/N at kHz frequencies. In this work, we have chosen to take into account only bone piezoelectricity because the stresses in the bones are much higher than those of other biological materials in and around the brain [127], and at this point we are mainly interested in order-of-magnitude estimates.

### 3.3 Three-dimensional blast-induced field simulation

Our general approach is to combine mechanical full-head simulations of an IED-scale blast wave with bone piezoelectric properties and an electrostatics solver, all using finite-element methods (FEM), to obtain the magnitude and distribution of typical in-brain electric fields, as schematically illustrated in Fig. 3-1. First, an incoming blast wave in the air hits the soldier's head—in our model system, the blast wave is...
incident from the side. Stresses are induced in the tissues in the head, and an electrical polarization is created via the bone piezoelectric effect as described in eq. (3.1) below, and this in turn is related to an induced charge density. From the charge densities and dielectric properties of various tissues, one can solve Poisson’s equation to determine the electric field everywhere in and around the head. The implementation of this procedure is complicated by the need to interpolate between different (but related) finite-element models for the mechanical and electrostatic simulations, as described below.

Note that the timescale of these fields is directly related to the timescale of the shock (as described in more detail below, the field is a linear function of the applied stresses, assuming a linear piezoelectric material). In particular, a typical IED explosion has a millisecond-scale high-pressure duration, and that is the value used here [127], which results in a ms-scale electric-field pulse, corresponding to kilohertz-scale (kHz) frequencies \( f \) (from the Fourier transform of a ms pulse), at which the wavelength \( c/f \) of light is hundreds of kilometers in air (and on the order of kilometers in brain matter where the refractive index is \( \sqrt{10^4} \) to \( \sqrt{10^5} \) [60]). Therefore, neither the wave nature of light nor induced magnetic fields are relevant on the scale of a human head: the electromagnetic response is accurately described by an electrostatic model in which purely electric fields are produced instantaneously in response to the charge density [86].

Now, there are two types of currents that can flow in the brain when it is subjected to an electric field — the free current \( J_f = \sigma_f E \) from the conductivity \( \sigma_f \), and the bound current \( J_b = \frac{\partial P}{\partial t} = \omega (\varepsilon - 1) E \triangleq \sigma_b E \) [86]. Plugging in some numbers, \( \sigma_b \approx 2\pi \cdot 1000 s^{-1} \cdot 8.85 \cdot 10^{-12} \text{ F/m} \cdot 10^5 \approx 0.005 \text{ A/Vm} \), which is 50 times smaller than \( \sigma_f = 0.28 \text{ A/Vm} \). To examine how significant the free current is, we calculate the skin depth of the field, which is given by \( \omega \sqrt{\mu \varepsilon / 2} \left( \sqrt{1 + \frac{\sigma_f^2}{\varepsilon_0 \omega^2}} - 1 \right)^{1/2} \approx 0.5 \text{ km} \) [96]. Since the skin depth is huge compared to the lengthscale of the head, we conclude that the free current conductivity is irrelevant to the field distribution in the brain.
Figure 3-2: The process of carrying out our simulation: 1. Taking the original stress data $\sigma$ at the nodes (shown in blue) of the FEM $M$ of the mechanical simulation. 2. Calculating the electric polarization $P$ on the nodes. 3. Computing the charge density $\rho$ at the midpoints of each element in $M$ by linearly interpolating $P$. 4. Performing Delaunay tetrahedralization on the midpoints of each element in $M$. The new nodes are shown in red and we denote the new mesh by $M'$. We then interpolate the dielectric property $\varepsilon$ from $M$ to $M'$.

### 3.3.1 Computational method

We start with a finite-element full-head-model [127] simulation of a typical IED-scale blast wave incident on an unhelmeted human head, as well as a human head protected by a kevlar helmet (Advanced Combat Helmet). These simulations employed a full-head tetrahedral mesh (denoted by $M$) in the context of a blast with an over-pressure of 30 atm (0.03 kbar): the 99% lethal dose ($LD_{99}$) for lung-injury survival in an unarmored person (albeit survivable with current personal-protection equipment), equivalent to 0.569 kg of TNT at a 0.6 m standoff distance. (As described in Ref. 127, the head model was generated with 1 mm$^3$ resolution from magnetic-resonance images [35] combined with a bone-windowed CT scan.) The computational head model differentiates 11 distinct biological materials (listed below) characterized by different mechanical properties such as nonlinear viscoelasticity, anisotropy, strong strain rate dependence, and relative dielectric permittivity. The simulation consists of fluid-solid interaction with a blast shockwave under open boundary conditions. In particular,
we obtain the stress tensor $\sigma$ in the bone regions.

Given the results of the FEM mechanical simulation, we must then construct a finite-element model of the electrostatic problem, by a process outlined in Fig. 3-2. To obtain the polarization by the piezoelectric effect from the stresses, we multiply $d$ by $\sigma$ according to eq. (3.1).

The piezoelectric coefficient $d$ is a rank-3 tensor (a “3D matrix”) encoding the polarization in response to different types and orientations of the stress. As we show in Sec. 3.4, the precise orientation and anisotropy of $d$ appear to make little difference in the resulting charge density in the skull from a blast wave (no more than a factor of 4) as long as the magnitudes of the components of $d$ are the same (technically, fixed Frobenius norm $||d||_F$). As long as the orientation does not vary too rapidly in space (since rapid oscillations in $d$ would yield canceling polarizations), the orientation is therefore not crucial in estimating the order of magnitude of the resulting electric field. Nevertheless, we consolidate the available experimental data to obtain a realistic piezoelectric tensor:

$$
\begin{bmatrix}
0 & 0 & 0 & 10.5 & -1.3 & 0 \\
0 & 0 & 0 & -1.3 & -10.5 & 0 \\
3.8 & 3.8 & 0.5 & 0 & 0 & 0
\end{bmatrix} \times 10^{-14} \text{C/N}
$$

(3.2)

where axes 1 and 2 are tangential to the plane of the skull and axis 3 is normal to the plane of the skull. Thus, these axes rotate relative to the location on the skull. For simplicity, we assume that the piezoelectric response in the skull is rotationally invariant around axis 3. (Here, we use the standard encoding of the rank-3 tensor $d$ as a matrix [21], where the six columns correspond to the six degrees of freedom in the symmetric stress tensor $\sigma$.) This piezoelectric tensor possesses rotational symmetry in the tangent plane of the skull. For the coefficients, we used values typical of those reported in a variety of measurements [7,24], where $d_{14} = 0.105 \text{pC/N}$ is the largest coefficient as reported by Ref. 24. The $d_{14}$ coefficient in femur corresponds to bending the bone along its length, and so we chose the corresponding coordinate system for the skull so that $d_{14}$ corresponds to bending the skull, and we assumed rotational
invariance with respect to bending around any axis in the tangent plane of the skull. Again, we will see that the precise arrangement of the coefficients in $d$ seems not to matter very much for the peak order of magnitude of the resulting in-brain electric field estimate.

Since the coordinate system of $\sigma$ is fixed in space, while the coordinate system of $d$ is skull-relative, we first rotate $\sigma$ into the skull-relative coordinate system for each location on the skull, and then rotate back the resulting $P$. This gives us the polarization vector $P$ (in the fixed coordinate system of $\sigma$) at each vertex of the finite-element model.

The electric polarization produces a local charge density $\rho$ via eq. (3.3) [86]:

$$\rho = -\nabla \cdot P. \quad (3.3)$$

We compute $\rho$ by linear interpolation of the polarization $P$ between the vertices of each tetrahedron (corresponding to first-order elements for $P$) in $M$ to obtain the charge density on the "dual" set of vertices located at the center of each tetrahedron, as shown in Fig. 3-2. Note that the combination of eq. (3.1) and eq. (3.3) means that not only large stresses but also large stress gradients give rise to large charge density $\rho$, which leads in Sec. 3.4 to large charge densities around small features such as eye sockets where there are large stress variations.

A new mesh is generated by Delaunay tetrahedralization and refinement (to ensure well-shaped tetrahedra) of these dual vertices using the free software TetGen [173], yielding a dual mesh $M'$. In order to obtain a finite computational volume, we truncate the mesh by a sphere of diameter 0.8 m (and we check convergence relative to this truncation radius as well as other refinement metrics below). Values of $\rho$ and $\varepsilon$ are interpolated onto $M'$ using TetGen from the original dual vertices of $M$. The tetrahedral elements of $M$ consist of eleven different zones: CSF (cerebrospinal fluid), eyes, glia, muscle, sinus, skin/fat, skull, venous (blood), ventricle, white matter, and gray matter. These zones are assigned dielectric values of 109, 1e5, 1e5, 3.5e5, 5, 4e4, 1e4, 5e3, 109, 4e4 and 1e5 respectively, using values from Ref. 58, Ref. 59, Ref. 60,
We then compute the electric potential $V$ by solving Poisson’s equation:

$$-\nabla \cdot (\varepsilon \nabla V) = \rho$$  \hspace{1cm} (3.4)

where $\varepsilon$ is the dielectric function, which varies through the different materials in different regions of the head as described above. We use a Galerkin discretization with first-order elements [126], via the libMesh finite-element library [95], to convert this into a real-symmetric positive-definite matrix equation that we solve by a conjugate-gradient method [74] with an incomplete-Cholesky preconditioner [64]. The most refined mesh that we employ below has $\gg 4$ million nodes and unknowns ($\gg 30$ million elements, show in Fig. 3-3).

Finally, since the electric field $\mathbf{E}$ is just $-\nabla V$, for first-order elements ($V$ linearly interpolated from values at the nodes), we obtain one electric-field value per element. We therefore compute $|\mathbf{E}|$ for each element and associate it with the center of that element (the dual vertices of $M'$). Typical electric fields at a given point in time during a blast wave for the unhelmeted case are shown in Fig. 3-7 and Fig. 3-8. In particular, we are mainly concerned with the $\mathbf{E}$ magnitudes in the brain regions (both white and gray matter) only, and this region is what is shown in our plots.

One of the important results of our calculation is the fraction of total brain volume with electric field magnitude $|\mathbf{E}| > 9$ V/m, i.e., 10 times the IEEE safety threshold [83]. We checked the convergence of this value with respect to both the outermost diameter of the simulation volume and also with respect to mesh resolution. Going from an outer diameter of 0.8 m to 6.4 m changed this value by less 0.2%. Doubling the spatial resolution in all of the high-field regions ($\gg 12$ V/m) and subsequently refining mesh quality (to ensure well-formed tetrahedra) changed this value by around 10%. This accuracy seems more than sufficient for our purposes, since we are mainly concerned with the typical order of magnitude and spatial distribution of the peak fields, and do not claim to know the material properties or blast conditions to better than order-of-magnitude precision.
3.3.2 Simple electric field estimation

As a simple check of our full numerical results, we make the approximation that the charge density in the skull locally resembles a sheet of charge. This allows us to estimate the field near the skull in these regions, because the field of a sheet of charge is known analytically, an approximation that should be valid close to the skull where the field is most intense. Therefore, we use this as a first approximation to estimate the maximum field magnitudes in the brain.

In particular, the electric field very close to a sheet of charge is insensitive to the finite size of the charged region, and therefore can be approximated by the known field of an infinite charged plane. In a uniform dielectric, that field has a magnitude $\rho_s/2\varepsilon$, where $\rho_s$ and $\varepsilon$ are the surface charge density and the permittivity of the material, respectively [86]. For a surface charge density at the interface between two materials with permittivities $\varepsilon_1$ and $\varepsilon_2$, it can be shown from the method of images [86], and taking the limit as the charges approach the interface from one side, that the corresponding field magnitude in both materials is $\rho_s/2\varepsilon_{\text{eff}}$ where $\varepsilon_{\text{eff}} = (\varepsilon_1 + \varepsilon_2)/2$ is the average permittivity. For the particular case of a volume charge density $\rho$ in a thin sheet of thickness $h$, the corresponding surface-charge density is $\rho_s = \rho h$. Therefore, we obtain the following estimate for the electric field magnitude near a charged region of the skull:

$$|\mathbf{E}| \approx \frac{\rho h}{2\varepsilon_{\text{eff}}}$$

(3.5)

$$\approx \rho h / \left(2\varepsilon_0 \frac{1 + 10^5}{2}\right)$$

(3.6)

$$\approx \rho \cdot 2300 \text{Vm}^2/\text{C}$$

(3.7)

where $\rho$ is the charge density, $h = 0.002$ m is the thickness of the skull, $\varepsilon_0 = 8.85 \cdot 10^{-12}$ F/m is the vacuum permittivity, and the relative permittivity $\varepsilon/\varepsilon_0$ of air and brain matter are 1 and roughly $10^5$ (at kHz frequencies [59]), respectively.
3.4 Results

We first consider the electric-field magnitude estimates in the brain obtained by simple charged-sheet (1D) electrostatic approximations.

Figure 3-4 displays the average and maximum charge density magnitude $|\rho|$ in the skull bone, as well as the corresponding estimated electric field with respect to time over the course of the blast-wave impact. An immediate observation is that $\rho_{\text{ave}} \ll \rho_{\text{max}}$, with the average $|\rho|$ being more than an order of magnitude smaller than the maximum $|\rho|$. This is consistent with the observation from Fig. 3-5 that high charge densities are often concentrated in small (cm-scale) regions. For example, we can see higher charge densities in the skull on the side facing the shockwave impact, both in the center of the side and also around the eye sockets where there are small features in the skull leading to large stress gradients (as mentioned in Sec. 3.3.1). The corresponding estimated maximum electric field from eq. (3.5) is 6 V/m. The peak charge density and estimated field are changed by less than 20% in the case of a helmeted head: a typical charge density for the helmeted case is shown in Fig. 3-6, and displays similar peak densities but over a smaller area of the cranium. This maximum field is attained in a millisecond-scale pulse (corresponding to the duration of the high-pressure blast front), and so should be compared to safety standards and medical procedures for millisecond-scale pulses (equivalent to the standards for kHz frequencies [83]). In particular, our estimated field magnitude on the order of 10 V/m is about an order of magnitude larger than the IEEE safety standards and are comparable to the electric fields used in rTMS, as reviewed in Sec. 3.1.

Next, we examine the results of our 3D finite-element electrostatics solver. There are several questions that one can address with these calculations: how large are the in-brain electric fields, how big a volume of the brain do the largest fields cover, and what is their spatial (and temporal) distribution in the brain? As discussed further below, we are mainly concerned here with typical orders of magnitudes, since the precise numbers will vary depending on the blast conditions and other uncertainties. As mentioned above, we derived our results from full-head simulations of a typical
IED-scale blast wave incident upon the head (both unhelmeted and helmeted) from the side [127]. The peak pressures and resulting fields occur over a ms-scale pulse [106], and in this section we display charge and field magnitudes at roughly the peak of this pulse.

As described above, from the mechanical pressure wave we first derive the charge density in the skull for an unhelmeted head, which is plotted from two perspectives in Fig. 3-5, with several labeled cross sections (A–D). From this, we solve for the resulting electric-field magnitude $|E|$, which is plotted from the same two 3D perspectives in Fig. 3-7(left) and for the cross sections A–D in Fig. 3-8 (along with the charge-density cross sections). As can be seen from these plots, $|E|$ reaches values of several V/m or more over localized regions of the brain close to the skull, and in fact reaches peak values of 18 V/m in volumes too small to be seen clearly in these plots. The volumes of these high-field regions are further quantified below. The largest fields are, not surprisingly, on the side of the head facing the impinging blast wave, but small regions of high field intensity appear elsewhere as well (e.g. near the top of the skull in Fig. 3-8. In all cases, however, the largest fields are within around 1cm of the skull, which is primarily the cerebral-cortex region that is responsible for many higher brain functions [13].

These calculations use a detailed head model for assigning the dielectric permittivity $\varepsilon$ to 11 different tissue zones throughout the head, as described in the previous section. This inhomogeneity plays a significant role in determining the electric field magnitude and distribution within the brain. To illustrate this point, we also computed the fields in a homogenized head model for comparison, with the same charge densities but with only three $\varepsilon$ materials: the outer skin/fat layer, bone, and with everything else assigned $\varepsilon = 10^5$ (the value for gray matter, which is larger than that of most other head materials such as white matter). The resulting $|E|$ distribution is plotted in Fig. 3-7(right), and is visibly smaller and less concentrated than for the full head model. Quantitatively, the peak $|E|$ is reduced to 12 V/m for the homogeneous-head model, and we show below that the volumes of high field magnitudes are also significantly reduced. Physically, regions of lower $\varepsilon$ in the full head model [such as
white matter \((10^4)\) or CSF \((10^2)\) increase \(|E|\) by producing surface charges at the boundaries between materials [86].

Rather than looking at peak fields, it is revealing to examine the volume of the brain that is exposed to fields over a given threshold. This is quantified in Fig. 3-9, which plots brain volume versus \(|E|\) threshold for the unhelmeted and helmeted heads for the detailed head \(\varepsilon\) model, and also for the unhelmeted head with the homogeneous \(\varepsilon\) model. From this plot, the helmet appears to have only minor benefit in reducing in-brain fields (explained in more detail below)—this is in line with the conclusions the helmet seems to have little benefit in terms of the mechanical effects of blast waves (although alternative helmet designs, e.g. with face masks, may have a larger effect [136]). As explained in the previous paragraph, a simplified homogeneous head model yields both smaller fields and smaller high-\(|E|\) volumes in Fig. 3-9. For the detailed head models, a volume of \(\approx 2.66 \cdot 10^5\) mm\(^3\) of the brain in the unhelmeted case, and \(\approx 2.21 \cdot 10^5\) mm\(^3\) of the brain in the helmeted case (83% of the unhelmeted case), are exposed to fields \(|E| > 0.3\) V/m, the IEEE safety standard for the general public [83]. Approximately \(2.2 \cdot 10^4\) mm\(^3\) and \(\approx 1.4 \cdot 10^4\) mm\(^3\) are exposed to fields exceeding the 0.9 V/m standard for controlled environments for the unhelmeted and helmeted cases respectively. (The helmeted case has a volume of \(\approx 63%\) of the unhelmeted case.) A brain volume of \(\approx 3.6\) mm\(^3\) for the unhelmeted case, and \(\approx 1.8\) mm\(^3\) for the helmeted case (50% of the unhelmeted case), are exposed to \(|E| > 9\) V/m, exceeding the IEEE threshold by an order of magnitude and reaching values comparable to rTMS [196]. Even smaller volumes are exposed to \(> 20\) V/m fields, but the interpretation of results in such small volumes is problematic because the underlying head model (derived from MRI scans) has only mm resolution.

As mentioned above, these results are best interpreted as typical orders of magnitude rather than as precise values, due to the variability of realistic blast circumstances and the uncertainties in the underlying model data. The blast circumstances in this particular simulation were chosen to have the typical orders of magnitude in amplitude and timescales, but of course actual blasts may vary significantly. There is also significant variability in the \(\varepsilon\) values of different tissue samples [58-60], and
these values also depend on the frequency (timescale) \([6,58-60]\), so while the \(\varepsilon\) values used here are typical orders of magnitude they may vary in practice. For comparison purposes, we have taken the lowest and highest possible dielectric value for each of the 11 zones of the head model among the measured data in Ref. 6,58-60 between 500 Hz and 2000 kHz (whereas our previous values were taken from data for 1000 kHz only), and performed the same analysis on the relationship between brain volume and \(|\mathbf{E}|\) threshold for the unhelmeted head. The results are shown in Fig. 3-9. The brain volume with fields with \(|\mathbf{E}| > 0.3 \text{ V/m} \approx 900 \text{ mm}^3\) for the low-dielectric case, and \(\approx 6.8 \cdot 10^5 \text{ mm}^3\) for the high-dielectric case; the brain volume with fields \(|\mathbf{E}| > 0.9 \text{ V/m}\) is approximately 30 \text{ mm}^3 for the low-dielectric case, and \(\approx 6.7 \cdot 10^4 \text{ mm}^3\) for the high-dielectric case. For \(|\mathbf{E}| > 9 \text{ V/m}\), the volume \(\approx 35 \text{ mm}^3\) for the low-dielectric case, and is identically zero for the high-dielectric case. First, it makes intuitive sense that lower dielectric permittivities imply a weaker shielding effect, and thus higher fields. The volumes for the high-dielectric case are of the same order of magnitude as in our original model, whereas in the high-dielectric case the brain volumes are apparently reduced by three orders of magnitude. However, when stretched by a factor of 10 in the \(|\mathbf{E}|\) axis, the high-dielectric curve overlaps almost exactly with the low-dielectric curve. This shows that our \(|\mathbf{E}|\) values are accurate as typical orders of magnitude, even after taking material property uncertainties into account.

Finally, we shall show that while the orientation of the piezoelectric tensor also matters, varying the overall orientation while keeping the magnitude fixed does not change the order of magnitude of the results [106]. As discussed above, we do not yet have experimental data on the piezoelectric response of human cranial bone, and are currently using typical values from other types of bone. There is some variation in measured data even for tibiae and femurs, and it is therefore worthwhile to investigate how sensitive the charge densities and resulting electric fields are to the precise details of \(\mathbf{d}\). Here, we assume that the orientation of the piezoelectric tensor is coherent (that the tensor orientation changes on the scale of at least centimeters, the lengthscale of coherence in our stresses and charge distributions), an assumption that has yet to be checked experimentally for the cranium but is consistent with measurements for
femurs and tibiae (which have a specific \( d \) orientation relative to the long axis of the bone). If \( d \) were rotating rapidly across the skull, then the polarizations would be pointing in different directions and could mostly cancel. We proceed with our sensitivity analysis. First, the charge density and electric field are clearly linear functions of \( d \) from eqs. (3.1) and (3.3), so simply multiplying \( d \) by a constant will scale \( \rho \) and \( E \) by the same constant. The only remaining question is the sensitivity with respect the “orientation” of \( d \): the distribution of the components of the \( d \) tensor with a fixed “average” magnitude. We quantify this by fixing the Frobenius norm \( \|d\|_F \) (the root-mean-square value of the components of \( d \)), imposing rotational symmetry in the tangent plane of the skull, and randomly varying the distribution of the components. We generate 100 random \( d \) tensors with this rotational symmetry, using a uniform distribution in \([-0.5, 0.5]\) to assign values to the non-zero degrees of freedom in the tensor and then rescaling to keep the norm \( \|d\|_F \) fixed to that of the tensor in eq. (3.2), and using these to calculate the charge densities as in Sec. 3.3.1. We show in Fig. 3-10 the histogram of the maximum charge density \(|\rho|\), and find that the maximum \(|\rho|\) varies by around a factor of 2–3 from the \(|\rho|\) produced by our original value of \( d \). Therefore, it seems that the precise details of the \( d \) orientation do not affect the order of magnitude of the charge density or the resulting in-brain electric fields.

3.5 Porcine skull piezoelectric measurements

Our collaborators, Ethan M. Parsons and Simona Socrate, have extended existing bone piezoelectricity measurement results by reporting new measurements of the piezoelectric response of bone under blast-wave conditions, using a split Hopkinson bar, for bovine femurs and porcine cranial bone, as shown in Fig. 3-12. They found that bovine femur samples (Fig. 3-11), when subjected to millisecond shocks, produce voltages consistent with previous constant-frequency measurements of bovine femurs [24]. These results are shown in Fig. 3-13. Porcine skull, on the other hand, exhibits no detectable piezoelectric response—a negative result that may stem from the
thick and spongy nature of porcine skull [12], in contrast to the hard thin cortical bone forming the structure of femurs as well as of human cranial bone [45, 122, 145, 146]. This variation in response between different types of bone makes it critical to obtain data in the future for human cranial bone in order to assess potential piezoelectric effects in response to blast waves.
Figure 3-3: Side view of one of the 3D finite-element meshes used in the Poisson simulation. A volume of 0.8 m diameter containing the head model is used. There are 5.8e6 nodes and 37e6 elements. This mesh is obtained by doubling the resolution of another mesh where $|E| > 12$ V/m.
Figure 3-4: Average and maximum piezoelectric charge density magnitude $|\rho|$ as a function of time, as well as the corresponding peak electric field estimate, over the course of a typical IED-scale blast impact for an unhelmeted human head.

Figure 3-5: Volume plots of charge densities in the skull for an unhelmeted head

[a] Volume charge density $\rho$ from the front

[b] Volume charge density $\rho$ from the side
Figure 3-6: Volume plots of charge densities in the skull for a helmeted head
Figure 3-7: Volume plots of electric field distribution in the brain for the full dielectric model and the homogeneous dielectric model.
Figure 3-8: Cross sections of charge densities in the skull and electric fields in the brain.
Figure 3-9: This is a plot of brain volume against the electric field magnitude threshold contained therein. The brain contains much lower fields if we assume a uniform dielectric of 1e5, which is the relative dielectric permittivity for gray matter. The presence of the helmet makes no noticeable difference.
Figure 3-10: Histogram of maximum charge densities calculated for 100 randomly oriented piezoelectric tensors. (The tensor components were chosen as uniform random numbers in $[-0.5, +0.5]$, and then $\mathbf{d}$ was rescaled to have a fixed Frobenius norm $\|\mathbf{d}\|_F = 0.159 \times 10^{-12}$ C/N.) The results show that the precise details of the piezoelectric orientation in cranial bone are unlikely to change the order of magnitude of the peak charge density, as long as the strength of the piezoelectric effect is the same.

Figure 3-11: Bovine femur specimens were cored in the axial direction from the distal end of the femur.
Figure 3-12: Bovine and cranial specimens were tested with the Split Hopkinson bar. Copper leads were attached to the radial surface of the specimen 180° apart.
3.6 Summarizing remarks

From our investigation, the biggest EM fields in the brain may come from an unexpected source – piezoelectricity of bone – that had not yet been studied in the context of blast TBI. Significant brain volume is found to have fields exceeding IEEE safety thresholds by an order of magnitude and comparable to rTMS procedures known to have neurological effects. This raises the possibility that piezoelectric fields produced by the blast waves impacting the skull may contribute to blast-induced TBI, a possibility that we believe merits further study. Future work should also consider the possibility that the effect of the electric fields on the brain is exacerbated by the mechanical blast injury, especially since increased intracranial pressure is already known to increase risks in rTMS [201].

There are a number of questions that should be addressed by future research. First, direct experimental measurements of shocked human cranial bone would be necessary to observe the resulting electric fields, determine the relevant piezoelectric coefficient, and compare with theoretical predictions. Future experimental measure-
ments of the piezoelectric effect in cranial bone should also determine any spatial variation of the piezoelectric coefficient $d$ across the thickness of the bone or in different regions of the skull; for example, any rapid variation in the magnitude or orientation of the piezoelectric tensor $d$ across sutures between cranial bones would lead to greatly increased $\rho$ at these joints.

Eventually, electromagnetic solvers may need to be directly coupled with shock-wave simulations. Ultimately, EM effects may need to be included in animal models and other research on blast-related TBI. Moreover, it would be desirable to have a more fully time-resolved simulation that takes into account material dispersion more carefully.

Regardless of whether piezo-induced electric fields play a role in blast-induced TBI, they may be useful in the research and diagnosis of blast-related injuries. In particular, the same mechanism that produces fields inside the brain also generates short-range fields of similar magnitudes immediately outside the head, and such kHz-frequency fields are easily measured by radio-frequency (RF) antennas. Small RF antennas incorporated into protective headgear could therefore provide a form of “blast dosimeter;” if the field strengths are recorded, they can be analyzed after the blast to provide a direct measure of the blast-induced stresses on the skull as a quantitative diagnostic metric [107].

**Appendix 3A: Ionization of air by IED blast waves**

In order to eliminate the possibility that ionization of air by the blast wave can itself lead to neurologically significant electric fields, we present a conservative order-of-magnitude estimate on thermodynamic grounds (suggested by E. Reed [154]). Here, we consider the ionization by the blast wave in air only, not the ionization within the detonation region (the initial flash). It turns out that the induced electric field in an air blast wave can be characterized in terms of the blast-wave pressure, temperature, and air-ionization energy alone, from thermodynamic considerations, independent of how the blast wave was generated, and we use these parameters to estimate the fields.
from an IED-scale blast below.

First, we estimate the electric field in terms of the charge density and temperature. An electric field from ionization must be created by the separation of charges, and this separation requires energy $qV$ where $q$ is the value of an individual charge (e.g., an electron) and $V$ is the voltage. This energy, if it is supplied by the blast wave, should be comparable to the thermal energy $kT$ where $k$ is Boltzmann’s constant and $T$ is temperature [157], assuming the charges equilibriate on a shorter timescale than the blast wave duration (milliseconds). If the blast wave has spatial width $\ell$ and the charge density is $\rho$, then the peak electric field will be $E \sim \rho\ell/\varepsilon_0$ (similar to eq. (3.5)) and the potential will be $V \sim E\ell \sim \rho\ell^2/\varepsilon_0$. Combining this with $qV \sim kT$ and solving for $\ell$, we obtain $\ell \sim \sqrt{kT\varepsilon_0/q\rho}$ and peak fields $E \sim \rho\ell/\varepsilon_0 \sim \sqrt{\rho k T / q \varepsilon_0}$.

Second, we obtain the charge density from the Boltzmann distribution: if the ionization energy of the gas is $I$ and the number density is $n$, then one should have $\rho = qne^{-I/kT}$ at equilibrium [157]. This can now be combined with the ideal gas law $P = nkT$ relating pressure $P$ to $n$ and $T$, and substituted into the above equation for $E$ to obtain:

$$E \sim \sqrt{\frac{Pe^{-I/kT}}{\varepsilon_0}}. \quad (3.8)$$

We now make a conservative estimate for $E$. Even if the temperatures in the blast wave were to reach $T = 1000$ K (0.086 eV) with pressures reaching $P = 100$ atm ($10^7$ Pa), with the ionization energy of air being $I \approx 10$ eV (slightly smaller than the typical value for gases [121]), this equation predicts electric fields of only $\sim 10^{-16}$ V/m. Recall, also, that any field produced in air is reduced in the brain by roughly a factor of the relative permittivity [86] of the brain tissue ($\sim 10^5$ [59]).

(For nuclear-scale blast waves with even higher temperatures in the thousands of K, the fields from ionization quickly become more significant, thanks to the exponential dependence in the Boltzmann factor $e^{-I/kT}$, and have been studied in more detail in that context. [63])
Appendix 3B: Procedures of computation

This section provides the detailed procedures of obtaining our results from the mechanical model from the Raul Radovitzky group.

First, we describe how to obtain the input files for the finite element simulation:

1. The mechanical simulation produces an input.tec file containing the stress tensors in the skull region only. These files are named similar to skull-0001880.tec, where the number is a time step in increments of 20, which represents about 4.6 milliseconds. There are also files named head-0001880.tec, which contain coordinates and stresses of the nodes, as well as a list of elements by the 11 zones of the head model (CSF, eyes, glia, muscle, sinus, skin/fat, skull, venous (blood), ventricle, white matter, and gray matter). There are 3 lines of header to each file, followed by coordinates and stress tensor components at each node. A list of the elements (4 numbers per element, denoting indices of the nodes in the element) in zone 1 follows. Then for each of the remaining 10 zones, there is a line stating which zone the following elements belong to and how many elements there are in the zone, followed by the list of elements.

2. We would like to obtain a file (filename).node of the coordinates of the center of each element in the skull region of the mechanical model and the associated charge density, along with an index, and use these points as part of the “dual mesh” of the Poisson simulation to solve for the electric fields. We run part_deriv_charge.py with input.tec as the input file, (filename).node as the output for the coordinates, and (filename).charge as the output file containing the charge density for each node whose coordinates are in (filename).node:

   ./part_deriv_charge.py input.tec (filename)

under the directory /home/kylkaren/Brain/dataProcessingFeb/

One could create these charge density files for more than one .tec file by modifying the script to use a loop (included but commented out) and suppressing the
need to take input and output file names as arguments. (tecplotReadWrite.py is used in part_deriv_charge.py, and can read .tec files with a single zone but not multiple zones. We shall come back to this in step 8.)

3. We need a simulation volume much larger than the head to have the property of air for the Poisson simulation. To create the surface of the sphere of this simulation volume, we can modify the radius \( R \) and meshing fineness \( l_3, l_2, \) and \( l_1 \) parameters (smaller = more fine) in /home/kylkaren/Brain/g-mesh/sphere.geo as desired, and in the same directory, run gmsh -3 sphere.geo -o boundary.msh

4. boundary.msh contains points on the surface of a sphere with radius and meshing fineness information as indicated above. There is some header information (5 lines) before the coordinates of the points, and surface information after the points. To include points from the spherical surface boundary.msh outside of the head into the new mesh, we use the sed command, which takes all the lines from line 6 to line \( (\text{numNodesSphere}+5) \):

\[
\text{sed -n '6, (numNodesSphere+5)p' (path/)boundary.msh | awk -F' ' '{print ($1+numNodes, $2, $3, $4)'} >> (filename).node}
\]

where numNodes is the number of nodes in (filename).node before this new addition of points, and numNodesSphere is the number of points in the spherical surface generated by gmsh. The purpose of the awk command is to make sure that the node indices are correct. It prints out the correct index, and the \( x, y, z \) coordinates into new columns in (filename).node. At this point, one would need to correct the header line of (filename).node by changing the first line to:

\[
\text{numNodes 3 1 0}
\]

where the 3 is to indicate that this is a three-dimensional mesh, and the 1 indicates that there is one scalar field other than the coordinates.
5. To connect the points in (filename).node to form a mesh, we perform Delaunay tetrahedralization by running TetGen, a free software for generating tetrahedral meshes [173], as follows:

```
tetgen (filename).node
```

(filename).1.node and (filename).1.ele files should be produced. (filename).1.node is essentially identical to (filename).node, and (filename).1.ele contains a header line

```
numEle 4 1 0
```

followed by the elements of the mesh, with each element indicated by the indices of the four nodes in it. numEle is the number of elements in the mesh. The 4 in the header line means that each element has four nodes. We now need to refine the mesh by “quality” factor (radius-edge ratio of the tetrahedra), in order that the tetrahedral elements have nice enough shapes for the Poisson simulation to be accurate. To refine the mesh by quality, we use the “-q” flag followed with no space by the desired quality. The default quality is 2.0, and a smaller number implies higher quality meshes. We will use 1.7 below. One can also specify the desired maximum tetrahedron volume by using the flag “-a” followed with no space. TetGen will optimize the meshing and try its best to meet these requirements. The “-r” flat indicates that this is a mesh refinement, “-V” stands for “verbose”, and “-C” checks the consistency of the final mesh.

```
tetgen -rVC -q1.7 (filename).1.node
```

The outfile files are (filename).2.node and (filename).2.ele. These files contain additional nodes and elements that are added for the refinement. This is the mesh for which we will solve the voltage at each node, and the electric field for each element. We denote this mesh by $M'$. 79
6. Before we can solve Poisson's equation, we need the dielectric property $\varepsilon$ and charge density $\varepsilon$ at each node of our new mesh $M'$—since we do not yet have these values for the points added during the refinement step above. Therefore, we need to interpolate $\varepsilon$ and $\rho$ values from the full dual mesh. We denote the full mesh with all the charge and dielectric property that we are interpolating from by $B$. We will first detail how mesh $B$ is created from three types of points, and then explain how we assign $\rho$ and $\varepsilon$ values to the nodes of $B$.

(a) Mesh $B$ is created from three types of nodes. First, we need the center point of every element in each of the 11 zones in the mechanical head model. As explained in step 1, head-000xxxx.tec files contain the elements on each of the 11 zones. The skull corresponds to zone 7, and we would like to obtain 10 other .tec files that can be read by tecplotReadWrite.py by running a script that extracts the relevant lines in the file and calculates the midpoint of each element. The script divideZones.py uses part_deriv_charge.py, and the latter can be modified to suppress the printing of the header line and calculation of the charge density (to save time, since in this case the charge density should be zero). We then run:

```bash
cp (filename).node (filename).b.node
./divideZones.py input.tec (filename).b.node
```

Now, the dual mesh points from the other 10 zones of the original head model in mesh $B$, stored in (filename).b.node

(b) The second type of nodes is a bit more subtle. The nodes and elements of the mechanical head model do not come with flags that indicates whether they are on the boundary of the head (outermost layer next to the air), and the head model is cut off slightly above the chin. To obtain a more accurate interpolation, a clear head/air boundary is needed, since mesh $B$ only contains points in the head and points farther away. Without this clear boundary, dielectric properties of the head region will “seep through” to the neighboring air points added by the refinement, rendering our results
inaccurate. I therefore added a second kind of points to mesh $B$ to denote the boundary in the negative $z$ direction: a plane normal to $z$ that is immediately below the lowest point of the head model, as well as some points surrounding the head close to this plane (approximately a very short and side cylinder), with the dielectric properties of air. To create the plane, we need to find out the lowest $z$ value of all the points in the original head model, $z_{\text{min}}$, and create a grid in the $xy$ plane at a $z$ value slightly below $z_{\text{min}}$:

`./createDielectric.py`

To obtain the "cylinder" around the base of the head, I examined the largest of the radius in the $xy$ plane of the head model for $z$ values towards the bottom of the head (in the script `createDielectric2.py`). Before running this script, I determine this range of $z$ values for which to make the cylinder by checking the skin/fat mesh in ParaView [105] to see where the skin/fat zone creases to define the head/air boundary, as $z$ decreases. To visualize a mesh in ParaView, one can run:

`tetgenVtu.py (someFile) numNodes numEle`

to convert `(someFile).node` and `(someFile).ele` from the TetGen format to `.vtu` format. These are created by running:

`./createDielectric2.py`

These points can be added to the $B$ mesh by typing:

`awk -F' ' '{print ($1+numNodesB, $2, $3, $4)}' plane`  
`>> (filename).b.node`

`awk -F' ' '{print ($1+numNodesB', $2, $3, $4)}' cylinder`  
`>> (filename).b.node`

where `numNodesB` and `numNodesB'` denote the number of nodes of $B$ before the addition of the new points in the given command. (These points can also be added to the Poisson simulation volume before step 5.)
(c) The third type of nodes in $B$ are points on the sphere of the simulation volume, which are assigned the properties of air. We described the generation of these points, which we added to mesh $M'$. We now add these to mesh $B$ as well:

```
sed -n '6, (numNodesSphere+5)p' (path/)boundary.msh | awk -F' ' '{print ($1+numNodesB'', $2, $3, $4}>> (filename).b.node
```

where `numNodesB''` is the number of nodes in $B$ before these points on the sphere have been added.

7. These boundary points from the plane and the cylinder in the above step, together with points in the “skin” region of the head model, comprise the head/air boundary. The skin/fat region (zone 6) of the original model consists of “skin” points on the surface of the entire head model, as well as “fat” points in regions like the cheek. It would be nice if future head models from the mechanical simulation had a mesh that distinguished between the outer skin layer and inner fat, but for now, to set a head/air boundary for interpolation purposes, I distinguished these two groups of points by checking whether each point in zone 6 is inside an ellipsoid inscribed in the head model that I generated by stretching points of a sphere (from `boundary.msh`) by different amounts in different directions, and shifting it around. TetGen was then used to generate the mesh from these points on the ellipsoid. The ellipse was changed by “trial and error” while checking against ParaView to make sure that it falls within a layer of skin. (For the check, the ellipse needs to be in the TetGen `.node` and `.ele` format, for viewing in ParaView, it needs to be in `.vtu` format. Again, `tetgenVtu.py` can be used for the conversion.) `pointL2bTest.cxx` under `/home/kylkaren/Brain/libmesh` is the file used to check if a given point is in the aforementioned ellipsoid. It uses the free finite-element `libMesh` library [95]. One runs:

```
make pointL2bTest
./pointL2bTest -d 3 (ellipse).node zone6.node
```
to check if the points in the skin/fat zone (zone6) are within the ellipsoid.

8. We now discuss how we assign dielectric properties to the various regions of mesh $B$. The “skin” nodes are assigned air properties while the inner “fat” nodes are assigned the property of fat for interpolation purposes. After we gather all the nodes for mesh $B$, these nodes can be connected by running TetGen. The charge density information (zero for anything not in the skull) is put in a .mtr file that consists of a single number $\text{numNodes}$ on the first line, and the list of values on subsequent lines. Dielectric properties of the 11 regions having values assigned from Ref. 6 as described earlier in this chapter. The above assignment of $\rho$ and $\varepsilon$ values is done by running:

./assignRhoEp.py

We are now ready to interpolate the scalar fields $\rho$ and $\varepsilon$ from the nodes of $B$ to the nodes of $M'$. The TetGen command for interpolating a scalar field onto .node file is:

```
tetgen -Pm " (someFile).node
```

where mesh $B$ needs to be in (someFile).b.node and (someFile).b.ele, and the scalar field to be interpolated must be in (someFile).b.mtr. This is taken care of by running:

./createHead.py

In our case, someFile=(filename). 2 Note that the $B$ mesh would need to be modified for new .tec input files, e.g., the nodes and elements of the head model become slightly displaced at each time point, and the geometries are therefore slightly different. The current files for interpolation with a simulation volume of diameter 0.8 m are located in

/home/kylkaren/Brain/dataProcessingFeb/Nov/bFiles/.

Please refer to createHead.py for details.
Our mesh for Poisson simulations along with relevant scalar field values are now ready. (filename).node contains all the nodes of $M'$ along with the associated $\rho$ and $\varepsilon$ values, and (filename).ele contains the elements.

9. After all the previous preparation steps, we can finally run the Poisson solver (written using the finite element library libMesh [95]) on the mesh. To do so, we change the output filename to (filename).Full.txt in secondTestNov.cxx, then do:

```
make secondTestNov
./secondTestNov -d 3 (filename).node
```

Now, the electric field for each element in our mesh in (filename).node and (filename).ele is given in the numEle lines of (filename).Full.txt for each element of $M'$, where numEle is the number of elements.

10. To extract the fields in the brain for plotting, we need to find out whether each element is in the brain or not, i.e., we need to sign a boolean value to the midpoint of each element in $M'$. This is done by running ./runDualMesh.py, which calculates the dual mesh of $M'$, and then interpolates an inBrain? boolean field from the $B$ mesh. We prepare the .mtr files as we did for $\varepsilon$ in step 8, except that we write a value of 1 for nodes of $M'$ that come from the white matter or gray matter zones in the original mechanical model, and 0 otherwise, instead of the dielectric values.

We also need to analyze the $E$ distribution in the brain volume, and this requires the calculation of the volume of each element in $M'$. The two tasks just mentioned are performed when we run ./runDualMesh.py via calling part_deriv_dualMesh.py. The outputs of runDualMesh.py are vol, a file containing the volumes of all the elements in $M'$, and inBrain.txt, a list of boolean values for the elements in $M'$. We can obtain the field in the brain for plotting by zeroing the fields that are not in the brain as follows:

```
paste vol inBrain.txt (filename).Full.txt >volBrainField
```
To obtain the in-brain field along with the volume of the corresponding element for analyzing the relationship between brain volume and electric field magnitude threshold, we extract the field in the brain elements along with the element volume, and obtain a list of total brain volume above various $|E|$ thresholds. After putting in relevant filenames in the script, we run:

```
awk -F' ' '{if ($2>0) print $1, ($2*$3)}'>fieldBrain2.txt

./averageVolBrain.py
```

The outputs from `averageVolBrain.py` can then be plotted using MATLAB.

11. To convert the file format of the output to .vtu for display in ParaView, run:

```
gmvVtu.py (filename) numNodes numEle
```

12. In the data visualization program ParaView, open originalMesh.vtu (the bone region of the original mechanical mesh with no data). Under “display”, choose “points”, and adjust the point size to 1.0 instead of the default 5.0. Change the opacity to 0.4. This is to be superimposed with the simulation results. To generate images of the 3D field (or charge), open the (filename).vtu, and choose “volume”. Note: These volume plots take quite some time to load, so don’t click on anything on the screen until it is completely finished loading; otherwise, ParaView will restart the process again.

After the plot loads, change the color scheme to the white-yellow-red-black bar for electric field plots, and adjust the scale as desired. Opacity in the low fields can be reduced to zero. For charge plots, use the blue-red plot, making white zero and zeroing the opacity for low absolute charge densities. Plots of the cross sections can be created by clicking on the toolbar. Make sure to uncheck the “eye” icon of the volume plot before doing so for time efficiency and to prevent overlapping images that do not go together.
13. To refine the mesh by doubling the resolution in high field regions, we add a point in every element with a field higher than a certain threshold:

`.refine2.py`

To ensure reasonable tetrahedral shapes, we refine by quality again using `tetgen -q...`, and interpolate values using `createHead.py` and `runDualMesh.py`. This prepares `.node` and `.ele` files refined by field for use in the next Poisson simulation.
Chapter 4

Localization theorems for guided modes in microstructured waveguides

In this chapter, we present two localization theorems regarding guided modes in microstructured waveguides. The first is a sufficient condition for the existence of index-guided modes in a very general class of dielectric waveguides, including photonic-crystal fibers (arbitrary periodic claddings, such as “holey fibers”), anisotropic materials, and waveguides with periodicity along the propagation direction. This condition provides a rigorous guarantee of cutoff-free index-guided modes in any such structure where the core is formed by increasing the index of refraction (e.g. removing a hole). It also provides a weaker guarantee of guidance in cases where the refractive index is increased “on average” (precisely defined below). The proof is based on a simple variational method, inspired by analogous proofs of localization for two-dimensional attractive potentials in quantum mechanics [109].

Generalizing the above condition to those required for two cutoff-free guided modes to exist, we obtain rigorous sufficient conditions for the existence of two cutoff-free index-guided modes in a wide variety of microstructured dielectric waveguides with arbitrary periodic claddings, based on the existence of a degenerate fundamental mode of the cladding (a degenerate light line). We show how such a degenerate light
line, in turn, follows from the symmetry of the cladding [108]. Conversely, we establish rigorous necessary analytical conditions for the existence of single-polarization single-mode (SPSM) bandwidths in index-guided microstructured waveguides. These conditions allow us to categorize designs for SPSM waveguides into four strategies, at least one of which appears to be previously unexplored.

Finally, we include the result of a localization theorem for bandgap guidance in quantum mechanics, in which 1D and 2D localization within the bandgaps of a periodic Schrödinger operator is shown for any mostly negative or mostly positive defect potential, $V$, whose depth is not too great compared to the size of the gap. This work was developed as an extension of our earlier ideas by A. Parzygnat, with my collaboration. Sufficient conditions for 1D and 2D localization below the ground state of such an operator are obtained in a similar way. Furthermore, our results are extended to 1D and 2D localization in $d$ dimensions, for example, by a linear or planar defect in a 3D crystal. For the case of $D$-fold degenerate band edges, we also give sufficient conditions for localization of up to $D$ states.

### 4.1 Rigorous sufficient conditions for index-guided modes in microstructured dielectric waveguides

In this section (from Ref. 109), we derive rigorous sufficient conditions for the existence of index-guided modes, including conditions for cutoff-free modes, in a wide variety of dielectric waveguides—from ordinary step-index fibers [180], to photonic-crystal “holey” fibers [15, 87, 162, 213], and even fiber-Bragg gratings [153] or other periodically modulated waveguides [44, 46, 87]. The dispersion relations of such waveguides must almost always be computed numerically, and so exact analytical theorems like the one derived here provide a foundation of certainty that is not available in any other way. A rigorous theorem allows us to give a general answer (although not a necessary condition) for questions such as: if the waveguide core has a mixture of higher- and lower-index regions, how much higher-index material is enough for cutoff-
free guidance; and under what conditions do photonic-crystal fibers, like step-index fibers, have cutoff-free guided modes. Our theorem provides an absolute guarantee, with no calculation required, that strictly increasing the refractive index to form the waveguide (e.g. filling in a hole of a holey fiber) yields a cutoff-free guided mode. Our work extends an earlier proof of guided modes for homogeneous-cladding, non-periodic, dielectric waveguides with isotropic [10] or anistropic [192] materials, and is closely related in spirit to proofs of the existence of bound modes in two-dimensional potentials for quantum mechanics [205].

The most common guiding mechanism in dielectric waveguides is index guiding (or “total internal reflection”), in which a higher-index core is surrounded by a lower-index cladding $\varepsilon_c$ ($\varepsilon$ is the relative permittivity, the square of the refractive index in isotropic non-magnetic materials). A schematic of several such dielectric waveguides is shown in Fig. 4-1. In particular, we suppose that the waveguide is described by a dielectric function $\varepsilon(x, y, z) = \varepsilon_c(x, y, z) + \Delta\varepsilon(x, y, z)$ such that: $\varepsilon$, $\varepsilon_c$, and $\Delta\varepsilon$ are

Figure 4-1: Schematics of various types of dielectric waveguides in which our theorem is applicable. Light propagates in the $z$ direction (along which the structure is either uniform or periodic) and is confined in the $xy$ direction by a higher-index core compared to the surrounding (homogeneous or periodic) cladding.

[a] Cross section of a waveguide (e.g. a conventional fiber) with a homogeneous cladding and an arbitrary-shape core.

[b] Cross section of a photonic-crystal fiber with periodic cladding and arbitrary-shape core.

[c] A waveguide periodic in the propagation ($z$) direction surrounded by a homogeneous cladding.
periodic in z (the propagation direction) with period a (a → 0 for the common case of a waveguide with a constant cross-section); that the cladding dielectric function \( \varepsilon_c \) is periodic in the \( xy \) plane (e.g. in a photonic-crystal fiber), with a homogeneous cladding (e.g. in a conventional fiber) as a special case; and the core is formed by a change \( \Delta \varepsilon \) in some region of the \( xy \) plane, sufficiently localized that \( \int |1/\varepsilon - 1/\varepsilon_c| < \infty \) (integrated over the \( xy \) plane and the unit cell in z). This includes a very wide variety of dielectric waveguides, from conventional fibers [Fig. 4-1(a)] to photonic-crystal “holey” fibers [Fig. 4-1(b)] to waveguides with a periodic “grating” along the propagation direction [Fig. 4-1(c)] such as fiber-Bragg gratings and other periodic waveguides. We exclude metallic structures (i.e, we require \( \varepsilon > 0 \)) and make the approximation of lossless materials (real \( \varepsilon \)). We allow anisotropic materials. The case of substrates (e.g. for strip waveguides in integrated optics [28,81,167]) is considered in Sec. 4.1.4. We also consider only non-magnetic materials (relative permeability \( \mu = 1 \)), although a future extension to magnetic materials should be straightforward.

Intuitively, if the refractive index is increased in the core, i.e. if \( \Delta \varepsilon \) is non-negative, then we might expect to obtain exponentially localized index-guided modes, and this expectation is borne out by innumerable numerical calculations, even in complicated geometries like holey fibers [15,87,162,213].

However, an intuitive expectation of a guided mode is far from a rigorous guarantee, and upon closer inspection there arise a number of questions whose answers seem harder to guess with certainty. First, even if \( \Delta \varepsilon \) is strictly non-negative, is there a guided mode at every wavelength, or is there the possibility of e.g. a long-wavelength cutoff (as was initially suggested in holey fibers [102], but was later contradicted by more careful numerical calculations [203]). Second, what if \( \Delta \varepsilon \) is not strictly non-negative, i.e. the core consists of partly increased and partly decreased index; it is known in such cases, e.g. in “W-profile fibers” [92] that there is the possibility of a long-wavelength cutoff for guidance, but precisely how much decreased-index regions does one need to have such a cutoff? Third, under what circumstances is it possible to obtain a “single-polarization” fiber, in which the waveguide is truly single-mode, rather than having two degenerate polarization modes as in a conventional cylindrical
fiber [43,99,112,123,138,175]? It turns out that all of these questions can be rigorously answered (in the sense of sufficient conditions for guidance) for the very general geometries considered in Fig. 4-1, without resorting to approximations or numerical computations.

We will proceed as follows. First, in Sec. 4.1.1, we review the mechanism of index guiding, state our result (a sufficient condition for the existence of index-guided modes), and discuss some important special cases. In Sec. 4.1.2, we first prove this theorem for the simplified special case of a homogeneous cladding $\varepsilon_c$, where the proof is much easier to follow. Then, in Sec. 4.1.3, we generalize the proof to arbitrary periodic claddings, such as for holey photonic-crystal fibers (with some algebraic details left to Appendix 4A). In Sec. 4.1.4, we discuss a few contexts that go beyond the initial assumptions of our theorem: substrates, material dispersion, and finite-size effects. We offer some concluding remarks in Sec. 4.1.5 discussing future directions.

**4.1.1 Statement of the theorem**

First, let us review the basic description of the eigenmodes of a dielectric waveguide [87,180]. In a waveguide as defined above, the solutions of Maxwell’s equations (both guided and non-guided) can be written in the form of eigenmodes $H(x, y, z)e^{i\beta z - \omega t}$ (via Bloch’s theorem thanks to the periodicity in $z$) [87], where $\omega$ is the frequency, $\beta$ is the propagation constant, and the magnetic-field envelope $H(x, y, z)$ is periodic in $z$ with period $a$ (or is independent of $z$ in the common case of a constant cross section, $a \to 0$). A plot of $\omega$ versus $\beta$ for all eigenmodes is the “dispersion relation” of the waveguide, one example of which is shown in Fig. 4-2. In the absence of the core (i.e. if $\Delta \varepsilon = 0$), the (non-localized) modes propagating in the infinite cladding form the “light cone” of the structure [15,87,162,213]; and at each real $\beta$ there is a fundamental (minimum-$\omega$) space-filling mode at a frequency $\omega_c(\beta)$ with a corresponding field envelope $H_c$ [15,87,162,213]. Such a light cone is shown as a shaded triangular region in Fig. 4-2. Below the “light line” $\omega_c(\beta)$, the only solutions in the cladding are evanescent modes that decay exponentially in the transverse directions [15,87,101,162,213]. Therefore, once the core is introduced ($\Delta \varepsilon \neq 0$), any new
solutions with $\omega < \omega_c$ must be guided modes, since they are exponentially decaying in the cladding far from the core: these are the index-guided modes (if any). Such guided modes are shown as lines below the light cone in Fig. 4-2: in this case, both a lowest-lying ("fundamental") guided mode with no low-frequency cutoff (although it approaches the light line asymptotically as $\omega \to 0$) and a higher-order guided mode with a low-frequency cutoff are visible. Since a mode is guided if $\omega < \omega_c$, we will prove the existence of a guided mode by showing that $\omega$ has an upper bound $< \omega_c$, using the variational (min–max) theorem for Hermitian eigenproblems [87].

Modes that lie beneath the light light are not the only type of guided modes in microstructured dielectric waveguides. While all the guided modes in a traditional, homogeneous-cladding fiber lie below the light line and are confined by the mechanism of index-guiding, there can also be bandgap-guided modes in photonic-crystal fibers [15, 87, 162, 213]. These bandgap-guided modes lie above the cladding light line and are therefore not index-guided. Bandgap-guided modes always have a low-
frequency cutoff (since in the long-wavelength limit the structure can be approximated by a "homogenized" effective medium that has no gap [178]). We do not consider bandgap-guided modes in this section; sufficient conditions for such modes to exist in the limit of large defect sizes were considered by Ref. 100. We consider the analogous quantum case in the limit of small defect sizes in Sec. 4.3.)

We will derive the following sufficient condition for the existence of an index-guided mode in a dielectric waveguide at a given \( \beta \): a guided mode must exist whenever

\[
\int \mathbf{D}_c^* \cdot (\varepsilon^{-1} - \varepsilon_c^{-1}) \mathbf{D}_c < 0,
\]

where the integral is over \( xy \) and one period in \( z \) and \( \mathbf{D}_c \) is the displacement field of the cladding's fundamental mode. From this, we can immediately obtain a number of useful special cases:

There must be a cutoff-free guided mode if \( \Delta \) is negative-definite everywhere (i.e., if we only increase the index to make the core, corresponding to \( \Delta \varepsilon \geq 0 \) for isotropic materials).

For a homogeneous cladding (and isotropic media), there must be a cutoff-free guided mode if \( \int (1/\varepsilon - 1/\varepsilon_c) < 0 \) (similar to the earlier theorem of Ref. 10, but generalized to include waveguides periodic in \( z \) and/or cores \( \Delta \varepsilon \) that do not have compact support).

More generally, a guided mode has no long-wavelength cutoff if eq. (4.1) is satisfied for the quasi-static (\( \omega \rightarrow 0, \beta \rightarrow 0 \)) limit of \( \mathbf{D}_c \).

Equation (4.1) can also be extended to a sufficient condition for having two guided modes (or, equivalently, a necessary condition for single-polarization guidance), when the cladding fundamental mode is doubly degenerate. We explore this generalization, analogous to a result in Ref. 10 for homogeneous claddings in Sec. 4.2.
4.1.2 Waveguides with a homogeneous cladding

To illustrate the basic ideas of the proof in a simpler context, we will first consider the case of a homogeneous cladding ($\varepsilon_c = \text{constant}$) and isotropic, $z$-invariant structures ($\varepsilon$ is a scalar function of $x$ and $y$ only). In doing so, we reproduce a result first proved (using a somewhat different approach) by [10] (although the latter result required $\Delta \varepsilon$ to have compact support, whereas we only require a weaker integrability condition). Our proof, which we generalize in Sec. 4.2, is closely inspired by a proof [205] of a related result in quantum mechanics, the fact that any attractive potential in two dimensions localizes a bound state [41,104,148,174,205]; we discuss this analogy in more detail below.

That is, we take the dielectric function $\varepsilon(x,y)$ to be of the form:

$$\varepsilon(x,y) = \varepsilon_c + \Delta \varepsilon(x,y), \quad (4.2)$$

where $\Delta \varepsilon$ is an arbitrary change in $\varepsilon$ that forms the core of the waveguide. For convenience, we define a new function $\Delta$ by:

$$\Delta(x,y) \triangleq \varepsilon^{-1} - \varepsilon_c^{-1}. \quad (4.3)$$

The only constraints we place on $\Delta \varepsilon$ are that $\varepsilon$ be real and positive and that $\int |\Delta| dx \, dy$ be finite, as discussed above. Now, we wish to show that there must always be a (cutoff-free) guided mode as long as $\Delta \varepsilon$ is "mostly positive," in the sense that:

$$\int \Delta(x,y) \, dx \, dy < 0, \quad (4.4)$$

Since eq. (4.4) is independent of $\omega$ or $\beta$, the existence of guided modes will hold at all frequencies (cutoff-free).

The foundation for the proof is the existence of a variational (min–max) theorem that gives an upper bound for the lowest eigenfrequency $\omega_{\text{min}}$. In particular, at each
\( \beta \), the eigenmodes \( \mathbf{H}(x, y)e^{i\beta z - i\omega t} \) satisfy a Hermitian eigenproblem \[^{[87]}\]:

\[
\nabla_\beta \times \frac{1}{\varepsilon}\nabla_\beta \times \mathbf{H} = \hat{\Theta}_\beta \mathbf{H} = \frac{\omega^2}{c^2} \mathbf{H}, \tag{4.5}
\]

where

\[
\nabla_\beta \triangleq \nabla + i\beta \hat{\mathbf{z}}, \tag{4.6}
\]

with eq. (4.5) defining the linear operator \( \hat{\Theta}_\beta \). In addition to the eigenproblem, there is also the “transversality” constraint \[^{[87,101]}\]:

\[
\nabla_\beta \cdot \mathbf{H} = 0 \tag{4.7}
\]

(the absence of static magnetic charges). From the Hermitian property of \( \hat{\Theta}_\beta \), the variational theorem immediately follows \[^{[87]}\]:

\[
\omega_{\text{min}}^2(\beta) = \inf_{\nabla_\beta \mathbf{H} = 0} Q(\mathbf{H}), \tag{4.8}
\]

where

\[
Q(\mathbf{H}) \triangleq c^2 \frac{\int \mathbf{H}^* \cdot \hat{\Theta}_\beta \mathbf{H} dx dy}{\int \mathbf{H}^* \cdot \mathbf{H} dx dy}. \tag{4.9}
\]

That is, an upper bound for the smallest eigenvalue is obtained by plugging any “trial function” \( \mathbf{H}(x, y) \), not necessarily an eigenfunction, into \( Q(\mathbf{H}) \) (the “Rayleigh quotient”, as defined above), as long as \( \mathbf{H} \) is “transverse” [satisfies eq. (4.7)]. [Technically, we must also restrict ourselves to trial functions where the integrals in eq. (4.9) are defined, i.e. the trial functions must be in the appropriate Sobolev space \( H(\nabla_\beta \times) \).]

Conversely, if eq. (4.7) is not satisfied, it is easy to make the numerator of the right-hand-side (which involved \( \nabla_\beta \times \mathbf{H} \)) zero, e.g. by setting \( \mathbf{H} = \nabla \varphi + i\beta \varphi \hat{\mathbf{z}} \) for any \( \varphi(x, y) \), so transversality of the trial function is critically important to obtaining a true upper bound.

Now, we merely need to find a transverse trial function such that the variational upper bound is below the light line of the cladding, which will guarantee a guided fundamental mode. For a homogeneous, isotropic cladding \( \varepsilon_c \), the light line is simply
\[ \omega_c^2 = \frac{c^2 \beta^2}{\varepsilon_c}, \]
and so the condition for guided modes becomes:

\[
\varepsilon_c \int \mathbf{H}^* \cdot \mathbf{H} dxdy - \beta^2 \int \mathbf{H} \cdot \mathbf{H} dxdy = \varepsilon_c \int \frac{1}{\varepsilon} \| \nabla \times \mathbf{H} \|^2 dxdy - \beta^2 \int \| \mathbf{H} \|^2 dxdy < 0, \quad (4.10)
\]

where in the second line we have integrated by parts. Although the basic idea of using the variational principle to estimate eigenvalues is well known, the challenge is to find an estimate that establishes localization even for arbitrarily small \( \Delta \varepsilon > 0 \) and/or for arbitrarily low frequencies.

The problem of bound states in quantum mechanics is conceptually very similar. There, given a potential function \( V(x, y) \) in two dimensions with \( \int |V| < \infty \), one wishes to show that \( \int V < 0 \) (attractive) implies the existence of a bound state: an eigenfunction of the Schrödinger operator \( -\nabla^2 + V \) with eigenvalue (energy) \( < 0 \). Again, this is a Hermitian eigenproblem and there is a variational theorem [34], so one merely needs to find some trial wavefunction \( \psi \) for which the Rayleigh quotient is negative in order to obtain a bound state. In one dimension, finding such a trial function is simple—for example, an exponentially decaying function \( e^{-\alpha|x|} \) (or a Gaussian \( e^{-\alpha^2} \)) will work for sufficiently small \( \alpha \)—and the proof is sometimes assigned as an undergraduate homework problem [189]. In two dimensions, however, finding a trial function is more difficult—in fact, no function of the form \( f(\alpha r) \) (where \( r \) is the radius \( \sqrt{x^2 + y^2} \)) will work (without more knowledge of the explicit solution for \( V \) [205]—and the earliest proofs of the existence of bound modes used more complicated, non-variational methods [41, 174]. However, an appropriate trial function for a variational proof was eventually discovered [10, 148], and a simpler trial function \( e^{-(r+1)\alpha} \) was later proposed independently by Yang and de Llano [205].

In the present electromagnetic case, we found that the following trial function, inspired by the quantum case above [205], works. That is, we can prove the existence of waveguided modes for a homogeneous cladding using the trial function, in cylindrical \((r, \phi)\) coordinates:

\[
\mathbf{H} = \mathbf{\hat{r}} \gamma \cos \phi - \mathbf{\hat{\phi}} (r\gamma)' \sin \phi, \quad (4.11)
\]
where

\[ \gamma = \gamma(r) = e^{1-(r^2+1)\alpha} \quad (4.12) \]

for some \( \alpha > 0 \), and \((r\gamma)'\) is the derivative with respect to \( r \). Clearly, \( H \) in eq. (4.11) reduces to an \( \hat{x} \)-polarized plane wave propagating in the \( \hat{z} \) direction as \( \alpha \to 0 \) (and hence \( \gamma \to 1 \)). This is a key property of the trial function: in the limit of no localization \((\alpha = 0, \Delta\varepsilon = 0)\) it should recover a fundamental (lowest-\( \omega \)) solution of the infinite cladding. Also, by construction, it satisfies the transversality condition (4.7) (which is why we chose this particular form). We chose \( \gamma \) slightly differently from Ref. 205 for convenience only (to make sure it is differentiable at the origin and goes to 1 for \( \alpha \to 0 \)). For future reference, the first two \( r \) derivatives of \( \gamma \) are:

\[ \gamma' = -2\alpha r (r^2 + 1)^{\alpha-1} \gamma, \quad (4.13) \]
\[ \gamma'' = 2\alpha (r^2 + 1)^{\alpha-1} \gamma \left[ -1 + 2\alpha r^2 (r^2 + 1)^{\alpha-1} + 2(1 - \alpha) r^2 (r^2 + 1)^{-1} \right], \quad (4.14) \]

and are plotted along with \( \gamma \) in Fig. 4-3.

What remains is, in principle, merely a matter of algebra to verify that this trial
function, for sufficiently small $\alpha$, satisfies the variational condition (4.10). In practice, some care is required in appropriately bounding each of the integrals and in taking the limits in the proper order, and we review this process below.

We substitute the trial function (4.11) for $H$ into the left-hand side of eq. (4.10):

$$\varepsilon_c \int \frac{1}{\varepsilon_c} \| (\nabla + i\beta \hat{z}) \times H(r, \phi) \|^2 d^2r - \beta^2 \int \|H\|^2 d^2r$$

$$= \varepsilon_c \int \left( \frac{1}{\varepsilon_c} + \Delta(r) \right) \left( \frac{1}{r} \left[ \frac{\partial}{\partial r} (rH_\phi) - \frac{\partial H_r}{\partial \phi} \right] + i\beta \hat{z} \times H \right) d^2r - \beta^2 \int \|H\|^2 d^2r$$

$$= \varepsilon_c \int \left( \frac{1}{\varepsilon_c} + \Delta(r) \right) \left( \frac{\sin^2 \phi}{r^2} \left\{ [r(r\gamma')]' - \gamma \right\}^2 + \beta^2 \|H\|^2 \right) d^2r - \beta^2 \int \|H\|^2 d^2r$$

$$= \varepsilon_c \int \left( \frac{1}{\varepsilon_c} + \Delta(r) \right) \frac{\sin^2 \phi}{r^2} (3r\gamma' + r^2\gamma')^2 d^2r + \varepsilon_c \int \beta^2 \Delta(r) \|H\|^2 d^2r$$

(4.15)

We proceed to show that the last line of the above expression is negative in the limit $\alpha \to 0$, thus satisfying the condition for the existence of bound modes. We first examine the second term of eq. (4.15):

$$\lim_{\alpha \to 0} \int \beta^2 \Delta(r) \|H\|^2 d^2r = \beta^2 \int \Delta(r) d^2r < 0.$$  

(4.16)

The key fact here is that we are able to interchange the $\alpha \to 0$ limit and the integral in this case, thanks to Lebesgue’s Dominated Convergence Theorem (LDCT) [75]: whenever the absolute value of the integrand is bounded above (for sufficiently small $\alpha$) by an $\alpha$-independent function with a finite integral, LDCT guarantees that the $\alpha \to 0$ limit can be interchanged with the integral. In particular, the absolute value of this integrand is bounded above by $|\Delta|$ multiplied by some constant (since $|H|$ is bounded by a constant: $|\gamma| \leq 1$ and $|r\gamma'|$ is also easily seen to be bounded above for sufficiently small $\alpha$), and $|\Delta|$ has a finite integral by assumption. Since $\lim_{\alpha \to 0} |H|^2 = 1$, we obtain eq. (4.4), which is negative by assumption.

Now we must show that the remaining first term of eq. (4.15) goes to zero as $\alpha \to 0$, completing our proof. This term is proportional to $\varepsilon_c^{-1} + \Delta$, but the $\Delta$ terms trivially go to zero by the same arguments as above: $\Delta$ allows the limit to be
interchanged with the integration by LDCT, and as \( \alpha \to 0 \) the \( \gamma' \) and \( \gamma'' \) terms go to zero. The remaining \( \varepsilon_c^{-1} \) terms can be bounded above by a sequence of inequalities as follows:

\[
\lim_{\alpha \to 0} \int_0^\infty \int_0^{2\pi} \frac{\sin^2 \phi}{r^2} (3r\gamma' + r^2\gamma'')^2 r \, d\phi \\
= 16\pi \lim_{\alpha \to 0} \int_0^\infty \alpha^2 r^3 (r^2 + 1)^{2\alpha-2} \gamma^2 \left[ -2 + \alpha r^2 (r^2 + 1)^{\alpha-1} + (1 - \alpha) r^2 (r^2 + 1)^{-1} \right]^2 \, dr \\
\leq 16\pi \lim_{\alpha \to 0} \int_0^\infty \alpha^2 r (r^2 + 1)^{2\alpha-1} \gamma^2 \left[ 2 + \alpha (r^2 + 1)^{\alpha} + (1 - \alpha) \right]^2 \, dr \\
= 16\pi \lim_{\alpha \to 0} \int_1^\infty \alpha^2 t^{4\alpha-1} e^{-2t^2\alpha} \left[ (3 - \alpha) + \alpha t^{2\alpha} \right]^2 \, dt \\
\leq 8\pi \lim_{\alpha \to 0} \int_0^\infty \alpha u e^{-2u} [(3 - \alpha) + \alpha u]^2 \, du \\
= 8\pi e^2 \lim_{\alpha \to 0} \alpha \left[ \frac{3}{8} \alpha^2 + \frac{1}{2} \alpha (3 - \alpha) + \frac{1}{4} (3 - \alpha)^2 \right] = 0.
\]

(4.17)

From the first to second line, we substituted eqs. (4.13) and (4.14) and simplified. From the second to third line, we bounded the integrand above by flipping negative terms into positive ones and replacing \( r^2 \) with \( r^2 + 1 \). From the third to the fourth line, we made a change of variables \( t^2 = r^2 + 1 \). Then, from the fourth to fifth line, we made another change of variable \( u = t^{2\alpha} \), and bounded the integral above by changing the lower limit from \( u = 1 \) to \( u = 0 \). The final integral can be performed exactly and goes to zero, completing the proof.

### 4.1.3 General periodic claddings

In the previous section we considered \( z \)-invariant waveguides with a homogeneous cladding and isotropic materials (for example, conventional optical fibers). We now generalize the proof in three ways, by allowing:

- transverse periodicity in the cladding material (photonic-crystal fibers),
- a core and cladding that are periodic in \( z \) with period \( a \) \( (a \to 0 \) for the \( z \)-invariant case),
anisotropic $\varepsilon_c$ and $\Delta \varepsilon$ materials ($\varepsilon$ is a $3 \times 3$ positive-definite Hermitian matrix).

In particular, we consider dielectric functions of the form:

$$\varepsilon(x, y, z) = \varepsilon_c(x, y, z) + \Delta \varepsilon(x, y, z), \quad (4.18)$$

where the cladding dielectric tensor $\varepsilon_c(x, y, z) = \varepsilon_c(x, y, z + a)$ is $z$-periodic and also periodic in the $xy$ plane (with an arbitrary unit cell and lattice), and the core dielectric tensor change $\Delta \varepsilon(x, y, z) = \Delta \varepsilon(x, y, z + a)$ is $z$-periodic with the same period $a$. Both $\varepsilon_c$ and the total $\varepsilon$ must be positive-definite Hermitian tensors. As defined in eq. (4.3), we denote by $\Delta$ the change in the inverse dielectric tensor. Similar to the isotropic case, we require that $\int |\Delta_{ij}|$ be finite for integration over the $xy$ plane and one period of $z$, for every tensor component $\Delta_{ij}$. We also require that the components of $\varepsilon_c^{-1}$ be bounded above.

In the homogeneous-cladding case, any light mode that lies beneath the (linear) light line of the cladding is guided. We have shown that such a mode always exists, for all $\beta$, under the condition of eq. (4.4), by showing that the variational upper bound on its frequency lies below the light line. In the case of a periodic cladding, the light line is the dispersion relation of the fundamental space-filling mode of the cladding, which corresponds to the lowest-frequency mode at each given propagation constant $\beta$ [15, 87, 162, 213]. This light “line” is, in general, no longer straight, and there are mechanisms for guidance that are not available in the previous case, such as bandgap guidance [15, 87, 162, 213]. Bandgap-guided modes may exist above the light line and are, in general, not cutoff-free because the gap has a finite bandwidth. Here, we only consider index-guided modes, which are guided because they lie below the light line. We will follow the same general procedure as in the previous section to derive the sufficient condition [eq. (4.1)] to guarantee the existence of guided modes. The homogeneous-cladding case is then a special case of this more general theorem, recovering eq. (4.4) (but generalizing it to $z$-periodic cores), where in that case the cladding fundamental mode $D_c$ is a constant and can be pulled out of the integral. The case of a $z$-homogeneous fiber is just the special case $a \to 0$, eliminating the $z$
The proof is similar in spirit to that of the homogeneous-cladding case. At each $\beta$, the eigenmodes $H(x, y, z)e^{i\beta z-\omega t}$ satisfy the same Hermitian eigenproblem (4.5) and transversality constraint (4.7) as before. We have a similar variational theorem to eq. (4.8) [87], except that, in the case of $z$-periodicity, we now integrate over one period in $z$ as well as over $x$ and $y$.

\[ \omega_{\min}^2(\beta) = \inf_{\nabla_\beta \cdot H = 0} Q(H) = \inf_{\nabla_\beta \cdot H = 0} c^2 \int H^* \cdot \hat{\Theta}_\beta H \int H^* \cdot H. \]  

As before, to prove the existence of a guided mode we will find a trial function $H$ such that this upper bound, the Rayleigh quotient for $H$, is below the light line $\omega_c(\beta)^2$. The corresponding condition on $H$ can be written [similar to eq. (4.10)]:

\[ \int H^* \cdot \hat{\Theta}_\beta H - \frac{\omega_c^2(\beta)}{c^2} \int H^* \cdot H < 0. \]  

We considered a variety of trial functions, inspired by the Yang and de Llano quantum case [205], before finding the following choice that allows us to prove the condition (4.20). Similar to eq. (4.11), we want a slowly decaying function proportional to $\gamma(r) = e^{1-(r^2+1)^\alpha}$, from eq. (4.12), that in the $\alpha \to 0$ (weak guidance) limit approaches the cladding fundamental mode $H_c$. As before, the trial function must be transverse ($\nabla_\beta \cdot H = 0$), which motivated us to write the trial function in terms of the corresponding vector potential. We denote by $A_c$ the vector potential corresponding to the cladding fundamental mode $H_c = \nabla_\beta \times A_c$. In terms of $A_c$ and $\gamma$, our trial function is then:

\[ H = \nabla_\beta \times (\gamma A_c) = \gamma H_c + \nabla \gamma \times A_c. \]  

For convenience, we choose $A_c$ to be Bloch-periodic (like $H_c$, since $A_c$ also satisfies a periodic Hermitian generalized eigenproblem and hence Bloch’s theorem applies). (Alternatively, it is straightforward to show that the Coulomb gauge choice, $\nabla_\beta \cdot A_c = 0$, gives a Bloch-periodic $A_c$, by explicitly constructing the Fourier-series components of $A_c$ in terms of those of $H_c$.) In contrast, our previous homogeneous-cladding trial
function [eq. (4.11)] corresponds to a different gauge choice with an unbounded vector potential \( \mathbf{A}_c = -\frac{1}{i\beta} \mathbf{y} + \nabla_\beta \psi \), differing from a constant vector potential via the gauge function \( \psi = \frac{r}{i\beta} \sin \phi + e^{-i\beta z} \).

Substituting eq. (4.21) into the left hand side of our new guidance condition (4.20), we obtain five categories of terms to analyze:

(i) terms that contain \( \Delta = \varepsilon^{-1} - \varepsilon_c^{-1} \),

(ii) terms that cancel due to the eigenequation (4.5),

(iii) terms that have one first derivative of \( \gamma \),

(iv) terms that have \( (\gamma')^2 \),

(v) terms that have \( \gamma'\gamma'' \) or \( (\gamma'')^2 \).

Category (i) will give us our condition for guided modes, eq. (4.1), while category (ii) will be canceled exactly in eq. (4.20). We show in Appendix 4A that all of the terms in category (iii) exactly cancel one another. The terms in categories (iv) and (v) all vanish in the \( \alpha \to 0 \) limit; we distinguish them because category (v) turns out to be easier to analyze. There are no terms with \( \gamma'' \) alone, as these can be integrated by parts to obtain category (iii) and (iv) terms. In Appendix 4A, we provide an exhaustive listing of all the terms and how they combine as described above. In this section, we only outline the basic structure of this algebraic process, and explain why the category (iv) and (v) terms vanish as \( \alpha \to 0 \).

Category (i) consists only of one term:

\[
\lim_{\alpha \to 0} \int \mathbf{H}^* \cdot (\nabla_\beta \times \Delta \nabla_\beta \times \mathbf{H}) = \int \mathbf{H}_c^* \cdot (\nabla_\beta \times \Delta \nabla_\beta \times \mathbf{H}_c)
\]

\[
= \int (\nabla_\beta \times \mathbf{H}_c)^* \cdot \Delta (\nabla_\beta \times \mathbf{H}_c)
\]

\[
= \frac{\omega_c^2}{c^2} \int \mathbf{D}_c^* \cdot \Delta \mathbf{D}_c
\]

(4.22)
From the first to the second line, we interchanged the limit with the integration, thanks to the LDCT condition as in Sec. 4.1.2, since the magnitudes of all of the terms in the integrand are bounded above by the tensor components \(|\Delta_{ij}|\) multiplied by some \(\alpha\)-independent constants, and \(|\Delta_{ij}|\) has a finite integral by assumption. (In particular, the \(A_c\) fundamental mode and its curls are bounded functions, being Bloch-periodic, and \(\gamma\) and its first two derivatives are bounded for sufficiently small \(\alpha\).) The result is precisely the left-hand side of eq. (4.1), which is negative by assumption.

Next, we would like to cancel \(-\frac{\omega_c^2}{c^2} \int \mathbf{H}^* \cdot \mathbf{H}\) by the eigen-equation (4.5). Thus, we examine the term \(\int \mathbf{H}^* \cdot \left( \nabla_\beta \times \varepsilon_c^{-1} \gamma \nabla_\beta \times \mathbf{H}_c \right)\) (which comes from the term where the right-most curl falls on \(\mathbf{H}_c\) rather than \(\gamma\)) below:

\[
\int \mathbf{H}^* \cdot \left( \nabla_\beta \times \varepsilon_c^{-1} \gamma \nabla_\beta \times \mathbf{H}_c \right) \\
= \int \mathbf{H}^* \cdot \left( \gamma \nabla_\beta \times \varepsilon_c^{-1} \nabla_\beta \times \mathbf{H}_c + (\nabla \gamma) \times \varepsilon_c^{-1} \nabla_\beta \times \mathbf{H}_c \right) \\
= \int \mathbf{H}^* \cdot \gamma \frac{\omega_c^2}{c^2} \mathbf{H}_c + \int \mathbf{H}^* \cdot \left( \nabla \gamma \times \varepsilon_c^{-1} \nabla_\beta \times \mathbf{H}_c \right) \\
= \int \mathbf{H}^* \cdot \frac{\omega_c^2}{c^2} \mathbf{H} - \int \mathbf{H}^* \cdot \frac{\omega_c^2}{c^2} \nabla \gamma \times \mathbf{A}_c + \int \mathbf{H}^* \cdot \left( \nabla \gamma \times \varepsilon_c^{-1} \nabla_\beta \times \mathbf{H}_c \right)
\]  

(4.23)

From the second to the third lines, we used the eigenequation (4.5), and from the third to the fourth lines we used the definition (4.21) of \(\mathbf{H}\) in terms of \(\mathbf{H}_c\). The first term of the last line above cancels \(-\frac{\omega_c^2}{c^2} \int \mathbf{H}^* \cdot \mathbf{H}\) in eq. (4.20). The second and third terms contain two category (iii) terms: \(\frac{\omega_c^2}{c^2} \int \gamma \mathbf{H}_c \cdot (\nabla_\gamma \times \mathbf{A}_c)\) and \(i\omega_c \int \gamma \nabla \gamma \cdot \mathbf{E}_c \times \mathbf{H}^*_c\), both of which will be exactly canceled as described in Appendix 4A, as well as some category (iv) and (v) terms.

The category (iv) integrands are all of the form \((\gamma')^2\) multiplied by some bounded function (a product of the various Bloch-periodic fields as well as the bounded \(\varepsilon_c^{-1}\)). This integrand can then be bounded above by replacing the bounded function with the supremum \(B\) of its magnitude, at which point the integral is bounded above by \(2\pi B \int_0^\infty (\gamma')^2 r \, dr\). However, such integrands were among the terms we already analyzed in the homogeneous-cladding case, in eq. (4.17), and we explicitly showed that such integrals go to zero as \(\alpha \to 0\).
The category (v) integrands could also be explicitly shown to vanish as \( \alpha \to 0 \), similar to eq. (4.17), but a simpler proof of the same fact can be constructed via the LDCT condition. In particular, similar to the previous paragraph, after replacing bounded functions with their suprema we are left with cylindrical-coordinate integrands of the form \( \gamma' \gamma'' r \) and \( (\gamma'')^2 r \). Both of these integrands, however, are bounded above by an \( \alpha \)-independent function with a finite integral, and hence LDCT allows us to put the \( \alpha \to 0 \) limit inside the integral and set the integrands to zero. Specifically, by inspection of eqs. (4.13) and (4.14), \( |\gamma' \gamma''| r < 4r^2(1+2+2)/(r^2+1)^2-\delta \) and \( (\gamma'')^2 r < 4r(1+2+2)/(r^2 + 1)^2-\delta \) for \( \alpha < \delta/4 \), and both of these upper bounds have finite integrals, if we take \( \delta \) to be some number \( < 1/2 \), since they decay faster than \( 1/r \).

In summary, we have shown that, if eq. (4.1) is satisfied, then the variational upper bound for our trial function [eq. (4.21)] is below the light line, and therefore an index-guided mode is guaranteed to exist. The special cases of this theorem, as discussed in the introduction, immediately follow.

4.1.4 Substrates, dispersive materials, and finite-size effects

In this section, we briefly discuss several situations that lie outside of the underlying assumptions of our theorem: waveguides sitting on substrates, dispersive (\( \omega \)-dependent) materials, and finite-size claddings.

An optical fiber is completely surrounded by a single cladding material, but the situation is quite different in integrated optical waveguides. There, it is common to have an asymmetrical cladding, with air above the waveguide and a low-index material (e.g. oxide) below the waveguide, such as in strip or ridge waveguides [28,81,167]. In such cases, it is well known that the fundamental guided mode has a low-frequency cutoff even when the waveguide consists of strictly nonnegative \( \Delta \varepsilon \) [28,81]. This does not contradict our theorem because we required the cladding to be periodic in both transverse directions, whereas a substrate is not periodic in the vertical direction.

We have also assumed non-dispersive materials in our proof. What happens when we have more realistic, dispersive materials? Suppose that \( \varepsilon \) depends on \( \omega \) but has
negligible absorption (so that guided modes are still well-defined). For a given \( \omega \), we can construct a frequency-independent \( \varepsilon \) structure matching the actual \( \varepsilon \) at that \( \omega \), and apply our theorem to determine whether there are guided modes at \( \omega \). The simplest case is when \( \Delta\varepsilon \geq 0 \) for all \( \omega \), in which case we must still obtain cutoff-free guided modes. The theorem becomes more subtle to apply when \( \Delta\varepsilon < 0 \) in some regions, because not only must one perform the integral of eq. (4.1) to determine the existence of guided modes, but the condition (4.1) is for a fixed \( \beta \) while the integrand is for a given frequency, and the frequency of the guided mode is unknown \textit{a priori}.

Finally, any real structure has a finite cladding. Both numerically and experimentally, this makes it difficult to study the long-wavelength regime because the modal diameter increases rapidly with wavelength (i.e. the frequency approaches the light line and the transverse decay rate becomes very slow)—in fact, it seems likely that the modal diameter will increase \textit{exponentially} with the wavelength. In quantum mechanics (scalar waves) with a potential well of depth \( V \), the decay length of the bound mode increases as \( e^{C/V} \) when \( V \to 0 \), for some constant \( C \) [174, 205]. In electromagnetism, for the long wavelength limit, a homogenized effective-medium \( \tilde{\varepsilon} \) description of the structure becomes applicable [178], and in this effective near-homogeneous limit the modes are described by a scalar wave equation with a “potential” \( -\omega^2 \Delta \tilde{\varepsilon} \) [86], and hence the quantum analysis should apply. Thus, by this informal argument, we would expect the modal diameter to expand proportional to \( e^{CA^2} \) for some constant \( C \) (where \( \lambda = 2\pi c/\omega \) is the vacuum wavelength), but a more explicit proof would be desirable.

4.1.5 Summarizing remarks

We have demonstrated sufficient conditions for the existence of cutoff-free guided modes for general microstructured dielectric fibers, periodic in either or both the \( z \) direction and in the transverse plane. The results are a generalization of previous results on the existence of such modes in fibers with a homogeneous cladding index. Our theorem allows one to understand the guidance in many very complicated structures analytically, and enables one to rigorously guarantee guided modes in many
structures (especially those where $\Delta \varepsilon \geq 0$ everywhere) by inspection. There remain a number of interesting questions for future study, however, some of which we outline below.

Our eq. (4.1) is a sufficient condition for index-guided modes, but it is certainly not necessary in general: even when it is violated, one can have guided modes with a cutoff (as for W-profile fibers [92] or waveguides on substrates [28,81]), or other types of guided modes (such as bandgap-guided modes [15,87,162,213]). However, these other types of guides modes in dielectric waveguides have a long-wavelength cutoff, so one can pose the question: is eq. (4.1) a necessary condition for cutoff-free guided modes (where $D_c$ is given by the long-wavelength limit of the cladding fundamental mode) in dielectric waveguides? In contrast, non-dielectric waveguides can also have cutoff-free guided modes, such as TEM modes in metallic coaxial waveguides [96]. Based on theoretical reasoning and some numerical evidence, we suspect that the answer is no, but that it may be possible to modify eq. (4.1) to obtain a necessary condition. In particular, the variational theorem is closely related to first-order perturbation theory: if one has a small perturbation $\Delta \varepsilon$ and substitutes the unperturbed field into the Rayleigh quotient, the result is the first-order perturbation in the eigenvalue. However, when $\Delta \varepsilon$ is large, even if the volume of the perturbation is small, perturbation theory requires a correction due to the electric-field discontinuity at the interface [90]. In the long-wavelength limit, perturbation theory is corrected by computing the quasi-static polarizability of the perturbation [90], and we conjecture that a similar correction to our trial field may allow one to derive a necessary condition for the absence of a cutoff. Equation (4.1) is still a sufficient condition (the variational theorem still holds even with a suboptimal trial function), but the preceding considerations predict that it will become farther from a necessary condition for the absence of a cutoff as $\Delta \varepsilon$ is increased, and this prediction seems to be confirmed by preliminary numerical experiments with W-profile fibers.

Also using a variational approach, Ref. 100 proved a sufficient condition for the existence of bandgap-guided modes in two dimensions. However, the condition established in that work was fairly strong, requiring a minimum defect size to guarantee
the existence of a guided mode, whereas numerical studies in one and two dimensions have suggested that no minimum defect size may be required [87], similar to the index-guided case proved here. If there is, in fact, no minimum defect size for gap-guided modes in linear defects, it is possible that a trial function similar to the one here could be applied to an approach like that of Ref. 100. While this has yet to be shown for the Maxwell's equations, our work has shown the analogous result for the Schrödinger operator Ref. 141, as we discuss in Sec. 4.3.5.

Let us also mention five other interesting directions to pursue. First, Ref. 10 actually proved a somewhat stronger condition than eq. (4.1) for homogeneous claddings, in that they showed the existence of guided modes when the integral was \( \leq 0 \) (and \( \Delta \epsilon > 0 \) in some region) rather than \( < 0 \) as in our condition. Although the \( = 0 \) case seems unlikely to be experimentally or numerically significant, we suspect that a similar generalization should be possible for our theorem (re-weighting the integrand to make it negative and then taking a limit as in Ref. 10). Second, as discussed in Sec. 4.1.4, it would be desirable to develop a sufficient condition at a fixed \( \omega \) rather than at a fixed \( \beta \), although we are not sure whether this is possible. Third, we would prefer a more rigorous version of the argument, in Sec. 4.1.4, that the modal diameter should asymptotically increase exponentially with the square of the wavelength. Fourth, it might be interesting to consider the case of “Bragg fiber” geometries consisting of “periodic” sequences of concentric layers [207], which are not strictly periodic because the layer curvature decreases with radius. Finally, as we mentioned in Sec. 4.1.1, it is possible to extend the theorem to a condition for two guided modes in many cases where the cladding fundamental mode is doubly degenerate, and the next section describes this result along with conditions for truly single-mode (“single-polarization”) waveguides.
4.2 Rigorous necessary conditions and design strategies for single-polarization single-mode waveguides

A single-polarization single-mode (SPSM) waveguide is a waveguide that is truly single-mode in the sense of supporting only a single guided-mode solution (rather than two or more, commonly corresponding to two polarizations as in standard “single-mode” fibers [153]); such waveguides are important, for example, as polarization-maintaining fibers (PMFs) [128]. (In contrast to a merely birefringent fiber, where two polarizations are guided but travel at different speeds [153], an SPSM fiber completely removes the possibility of coupling one polarization into the other.) In this section (from Ref. 108), we derive rigorous necessary conditions to obtain SPSM waveguides, and identify different categories of such designs, especially focusing on those that yield cutoff-free single-polarization regions with isotropic materials (compared to most previous designs that either employ birefringent materials or have long-wavelength cutoffs in both polarizations). The latter categories require an inhomogeneous fiber cladding, such as in a photonic-crystal fiber (a periodic cladding), as opposed to traditional dielectric waveguides surrounded by asymptotically homogeneous cladding materials. More specifically, generalizing the results from the previous section that derived sufficient conditions for index-guided modes in microstructured dielectric waveguides [109] as well as an earlier theorem for homogeneous-cladding waveguides [10,192], we derive sufficient conditions for a dielectric waveguide to support two index-guided modes when the cladding has a doubly degenerate light-line mode (usually as a consequence of symmetry). This is an entirely analytical result that provides rigorous guarantees for a wide range of microstructured waveguide geometries. In consequence, we are able to categorize single-polarization waveguides into four categories: (i) those that violate the conditions of our theorem entirely, typically resulting in a cutoff for both polarizations; (ii) those that employ anisotropic materials to guide one polarization and not the other; (iii) those using an asym-
metrical cladding structure (e.g. an asymmetrical photonic crystal) that does not have a doubly degenerate light-line mode; and (iv) those with a symmetrical periodic cladding that exploit the asymmetry of the light-line's two polarizations to guide one polarization but not the other. Most previous single-polarization designs fall into category (i) \[29, 42, 47, 51, 91, 99, 111, 112, 114, 123, 137, 138, 165, 175, 185, 187, 208, 212\] (also including non-index-guiding structures such as coaxial metallic guides \[197\]) or category (ii) \[30, 31, 43, 161, 181, 212\], and we will give examples of designs in categories (iii) \[94, 115, 183\] and (iv).

In a perfectly cylindrical fiber, the fundamental mode is doubly degenerate and there are two orthogonal “polarizations” with the same dispersion relation, and hence travelling at the same velocity down the fiber. Due to mechanical and thermal stresses induced during the fabrication process and by environmental conditions, there is often a slight asymmetry in the fiber geometry, which breaks the degeneracy of the two polarization modes \[153\]. The two modes then travel at slightly different velocities, causing pulse broadening via polarization-mode dispersion (PMD) \[153\]. Polarization-maintaining (PM) fibers \[128\] are optical fibers that can faithfully preserve and transmit the polarization state of the light that is launched into it under practical operating conditions, to alleviate the problem of PMD and provide a known polarization output at the end face of the fiber (useful for coupling to polarization-sensitive devices such as most integrated optics). Effectively single-polarization behavior can also be observed in hollow metallic tubes \[119\] and in photonic-bandgap fibers, both of which can operate in a non-degenerate lowest-loss mode (e.g. the \(\text{TE}_{01}\) mode) \[88\]—even when these waveguides are multimode, the higher loss of the other modes effectively filters them out. The strictest guarantees of polarization maintenance, however, are achieved in SPSM fibers, in which only one polarization mode is guided, rather than having two (or more) guided polarization modes that are merely birefringent and difficult to convert between.

To be more precise, the two “polarizations” merely refer to the two lowest-frequency guided modes. They may or may not correspond to two orthogonal linear polarizations, and may or may not be degenerate. The terminology came about from the
scalar limit: in conventional homogeneous-cladding fibers, the core has a very slightly increased index from the cladding, and in this “weakly-guiding” limit, the scalar approximation [180] applies and the two lowest-frequency solutions are purely polarized in two orthogonal directions [87, 180] (known as the “linearly polarized” LP01 modes [180]). (The scalar approximation applies in the high-frequency limit to holey fibers as well [14, 18, 87].) More generally, the two lowest-frequency modes are two linearly independent guided-mode solutions that satisfy the usual field-orthogonality relationships [87, 180], but are neither purely polarized in one direction nor are 90° rotations of one another (e.g. in a holey fiber with sixfold-symmetry). With sufficient symmetry, the two “polarization” solutions are degenerate [184]. We shall return to the details of the effect of symmetry on the structure of the guided modes in the subsequent discussion.

In Sec. 4.2.1, we first derive rigorous sufficient conditions to obtain two cutoff-free guided modes in a wide range of microstructured fibers. In many cases, these conditions allow one to rigorously predict the existence of two guided “polarizations” without calculation, merely from the fact that the waveguide core was created by strictly increasing the refractive index. This theorem depended on the existence of a doubly degenerate space-filling fundamental mode of the waveguide cladding (in the absence of the waveguide core), and in Sec. 4.2.2 we discuss under what conditions this degeneracy follows from the symmetry of the cladding. The contrapositive of our sufficient conditions for two guided modes are necessary conditions for SPSM waveguides, and in Sec. 4.2.3 we apply these necessary conditions to divide old and new designs for SPSM waveguides into four categories. We discuss and give examples of each of these categories in Sec. 4.2.4 through Sec. 4.2.7. Finally, we conclude in Sec. 4.2.8 with some remarks about open questions and future directions.

4.2.1 Two-polarization waveguides

In this section, we will derive and discuss sufficient conditions for a waveguide to have at least two linearly independent index-guided modes. (The contrapositive of this will be necessary conditions for a single-polarization waveguide, which are discussed
in Sec. 4.2.3.) These sufficient conditions are a generalization of our proof of the existence of at least one index-guided mode under certain conditions in Sec. 4.1 [109].

A dispersion relation of a three-dimensional waveguide is shown in Fig. 4-4. The guided modes are shown as lines below the light cone in Fig. 4-4: in this case, both a lowest-lying ("fundamental") guided mode with no low-frequency cutoff (although it approaches the light line asymptotically as $\omega \to 0$) and higher-order guided modes with low-frequency cutoffs are visible. In this particular case, there are actually two non-degenerate cutoff-free guided modes corresponding roughly to two polarizations; the fields are not purely polarized, so the two polarizations can be more precisely distinguished in terms of their even/odd symmetry with respect to the mirror planes of the waveguide [87].

In many important cases, the cladding fundamental mode $\omega_c(\beta)$ is doubly degenerate (two linearly independent "polarizations" with the same frequency $\omega_c$)—this is independent of whether the guided mode is doubly degenerate, which depends on the symmetry of the core as well as of the cladding. When $\omega_c$ is doubly degenerate,
one obtains an index-guided mode if eq. (4.1) is true for any of the degenerate fundamental modes $D_c$ (because any one of these modes could have been used in the proof from Ref. 109). If eq. (4.1) holds for all of the degenerate fundamental field patterns $D_c$, then one is guaranteed to have at least two index-guided modes (a two-polarization waveguide). We now prove this statement, a generalization of a result in Ref. 10 for homogeneous claddings. In the subsequent section, we will give symmetry conditions to have a doubly degenerate light line $\omega_c$, but here we simply assume that to be the case.

The variational theorem [eq. (4.19)] gave us an upper bound for the lowest-frequency mode’s $\omega$ in terms of the Rayleigh quotient $Q(H)$ for any divergenceless trial function $H$. In order to obtain an upper bound for the $n$-th mode’s frequency $\omega_n$, the variational theorem can be generalized as follows [10]:

$$\omega_n^2 \leq \sup_{H \in \mathcal{H}_n} Q(H),$$

(4.24)

where $\mathcal{H}_n$ is any $n$-dimensional subspace of divergence-free vector fields. That is, the supremum of the Rayleigh quotient of any $n$-dimensional subspace is an upper bound for the $n$-th eigenfrequency. Equality is achieved when $\mathcal{H}_n$ is the span of the $n$ lowest-$\omega$ modes, and for this subspace the maximum of the Rayleigh quotient is $\omega_n^2$.

The consequence of eq. (4.24), here, is that if we can find any two-dimensional subspace $\mathcal{H}_2$ of divergence-free trial fields such that $Q(H)$ is below the light line for every field $H$ in the subspace, then the second eigenfrequency $\omega_2$ must also lie below the light line, and hence there must be two guided modes. We can find such a subspace, assuming that the fundamental mode $H_c$ (and $D_c$) of the cladding is doubly degenerate, if eq. (4.1) is satisfied for both degenerate modes and all their linear combinations. We construct the subspace $\mathcal{H}_2$ as follows. Given two linearly independent cladding fundamental modes $H_c^{(1)}$ and $H_c^{(2)}$, we construct the corresponding trial functions $H^{(1,2)}$ as in Ref. 109. Because this construction is linear, $H = c_1 H_c^{(1)} + c_2 H_c^{(2)}$ is then the trial function constructed from $H_c = c_1 H_c^{(1)} + c_2 H_c^{(2)}$ for any constants $c_1$ and $c_2$. Because $H_c$ is also a cladding fundamental mode, and satisfies eq. (4.1) by as-
sumption, then $Q(H) < \omega_c^2$ by exactly the same proof as in Ref. 109. Hence $Q < \omega_c^2$ for every $H$ in $\mathcal{H}_2 = \text{span}\{H^{(1)}, H^{(2)}\}$, and there are at least two index-guided modes. Given a doubly-degenerate cladding fundamental mode $H_c^{(1,2)}$, it is not in general sufficient for eq. (4.1) to be satisfied only for any two of these modes; it must be satisfied for all their linear combinations as assumed above. The reason is that, given the displacement fields $D_c^{(1,2)}$ and some linear combination $D_c = c_1 D_c^{(1)} + c_2 D_c^{(2)}$, when substituted into eq. (4.1) there are cross terms $2\Re \left[ \int (D_c^{(1)})^* \cdot \Delta D_c^{(2)} \right]$ that may be positive. On the other hand, if eq. (4.1) holds for two degenerate cladding fundamental modes that one has orthogonalized in the sense that $\int (D_c^{(1)})^* \cdot \Delta D_c^{(2)} = 0$, then it holds for all linear combinations and the existence of at least two index-guided modes follows.

The easiest case, of course, is the one in which $\Delta$ is nonpositive-definite (e.g. if $\Delta \varepsilon \geq 0$ everywhere), in which case eq. (4.1) always holds. As we will describe below, a holey photonic-crystal fiber with sufficient symmetry always has a doubly-degenerate fundamental cladding mode, and it follows that filling in a hole (or otherwise strictly increasing $\varepsilon$) will always result in two cutoff-free index-guided modes (which are also degenerate if the core has sufficient symmetry, but may be nondegenerate otherwise).

Another simple common case is the one in which all degenerate modes have the same displacement-field magnitude $|D_c|$ everywhere—this is true for a homogeneous cladding (where $|D_c|$ is a constant), and also for an arbitrary cladding in the large-$\beta$ limit where a scalar approximation becomes valid [14, 18, 87]. Then, if the materials are isotropic, so that $\int D_c^* \cdot \Delta D_c = \int \Delta |D_c|^2$, eq. (4.1) will hold for all degenerate modes (if it holds for any of them) and one is guaranteed two index-guided modes. (This reproduces the result proved by Ref. 10 for homogeneous claddings.)

In general, $|D_c|$ is not the same for different degenerate modes of an inhomogeneous cladding. However, if the degeneracy is due to cladding symmetry as described below, and the core $\Delta \varepsilon$ preserves this symmetry, then eq. (4.1) is equivalent for all degenerate modes. That is, in symmetric structures (with three-fold, four-fold, or six-fold symmetry as described below), it is sufficient for eq. (4.1) to hold for one of the degenerate modes, from which it follows that it holds for all of the degenerate
[a] Three-fold symmetry $C_{3v}$.  
[b] Four-fold symmetry $C_{4v}$.  
[c] Six-fold symmetry $C_{6v}$.  
[d] Cylindrical symmetry $C_{\infty v}$.

Figure 4-5: Example microstructured optical fiber cladding structures with three-fold, four-fold, six-fold and cylindrical rotation symmetries. Claddings with these symmetries are guaranteed to have a doubly-degenerate light line, at least in the long-wavelength limit for cases [a–c].

modes. (The reason for this is that $\int \mathbf{D}_c^* \cdot \Delta \mathbf{D}_c$ is invariant under symmetry operations/rotations of $\mathbf{D}_c$ if $\Delta$ is invariant and hence commutes with the rotation.) In this case, again, one is guaranteed at least two index-guided modes in the (symmetric) core, and in fact these two modes must themselves be doubly degenerate (because they cannot be orthogonal to the trial functions, and hence cannot belong to a different irreducible representation). So, for example, a typical holey fiber formed by a triangular lattice of circular air holes (with six-fold symmetry) and a missing-hole waveguide core [87] is guaranteed analytically to have a degenerate pair of cutoff-free index-guided modes.

### 4.2.2 Symmetry and the degeneracy of the light line

Under what conditions is the cladding fundamental mode doubly degenerate? Usually, such degeneracy is a consequence of symmetry, and in particular is a consequence of the cladding symmetry group having a two-dimensional irreducible representation [85, 87, 184]. (Any degeneracy that does not result from symmetry is known as “accidental,” but this is something of a misnomer since accidental degeneracies are very unlikely to arise by chance [190].) For example, two-dimensional irreducible representations arise when the cladding has three-fold ($C_{3v}$), four-fold ($C_{4v}$), or six-fold
Figure 4-6: First two bands (Bloch modes) of a holey-fiber cladding (triangular lattice, period $a$, of radius 0.3$a$ air holes in index-1.45 silica) plotted around the boundary of the irreducible Brillouin zone (inset). Each pair of bands is plotted for a fixed value of $\beta$: $\beta = 0.001, 0.2, 0.5, \text{ and } 1.0$ in units of $2\pi/a$. The bands are doubly degenerate, by symmetry, at the $\Gamma$ point, and, because this is the lowest-frequency mode at each $\beta$, it is the (doubly degenerate) fundamental mode of the cladding and defines the light line.

$(C_{6v})$ symmetry [85], as depicted schematically in Fig. 4-5[a–c]. Even if the symmetry group has a two-dimensional representation, this would not seem to guarantee that the fundamental mode will fall into this representation and be doubly degenerate, but it is easy to check whether this is the case by a small calculation using the unit-cell of the cladding—in particular, the common “holey fiber” claddings of a square or triangular lattice of symmetrical air holes in dielectric both have doubly degenerate fundamental cladding modes. Also, in the common case of a homogeneous, isotropic cladding ($C_{\infty v}$ symmetry), the cladding fundamental mode is known analytically to be the two orthogonal linear polarizations (which fall into a two-dimensional irreducible representation).

However, by considering the relationship between an arbitrary periodic (symmetrical) cladding and the homogeneous case more carefully, it turns out that there is a guarantee that a sufficiently symmetrical cladding (one with a two-dimensional ir-
reducible representation) will have a doubly degenerate fundamental mode for all sufficiently long wavelengths. This guarantee is implied by continuity considerations for the eigenmode’s irreducible representation, which force the fundamental-mode symmetry to be determined by the long-wavelength quasi-static limit. As an example to illustrate this argument, consider the fundamental mode of the typical holey fiber cladding, a triangular lattice of air holes in silica, which is plotted in the cladding Brillouin zone [87] for several values of $\beta$ in Fig. 4-6. As $\beta$ goes to zero, the fundamental mode at the $\Gamma$ point must go to zero frequency: this is the long-wavelength “quasi-static” solution, and in this limit the structure can be replaced by an effective homogeneous medium [178]. Moreover, the rotational symmetry of the structure implies that the effective homogeneous medium must be isotropic, and hence must have a doubly degenerate fundamental mode consisting of two orthogonal polarizations. But two orthogonal polarizations are described by one of the two-dimensional irreducible representations of the six-fold symmetry group [85], which means that the exact solution at $\Gamma$ must also fall into this representation. The reason is that, as $\beta$ is increased and the $\Gamma$-point mode moves up in frequency, the corresponding field pattern must change continuously—it cannot discontinuously jump from one symmetry representation to another. Therefore, as long as the fundamental mode is the mode at the $\Gamma$ point, it must be doubly degenerate. The only way that the fundamental mode could conceivably become non-degenerate would be if, for some sufficiently short wavelength, the frequency at some other point in the Brillouin zone (e.g. M or K) became lower than the frequency at $\Gamma$. It may be that this is possible, although we do not observe it to occur for this structure. Regardless, the conclusion remains that, at least for sufficiently long wavelengths (once the $\omega$ at $\Gamma$ becomes the lowest), the cladding fundamental mode must be doubly degenerate. The same conclusion holds for every other crystalline symmetry group (three-fold, four-fold, or six-fold symmetry) in which there is a two-dimensional irreducible representation.
4.2.3 Four strategies to design SPSM waveguides

Above, we derived a sufficient condition to have two linearly independent guided modes in the waveguide. The contrapositive of this is a necessary condition to have only a single guided mode: one must violate the conditions of the theorem to obtain such a waveguide. This is a useful result, because truly single-polarization single-mode (SPSM) waveguides are the most robust way to obtain a polarization-maintaining waveguide, and have been proposed by many authors for this application [29–31,42,43, 47,51,91,94,99,111,112,114,115,123,137,138,161,165,175,181,183,185,187,208,212].

One can divide the mechanisms for violating the conditions for two-mode guidance into four strategies for single-polarization waveguides:

(i) Violate eq. (4.1) entirely, or the underlying conditions of the theorem (e.g. employ a non-periodic cladding, such as an asymmetrical substrate). With one notable exception, this typically means that both polarizations have cutoffs for index-guiding, where the cutoffs are different because of some asymmetry and hence there is a single-polarization region.

(ii) Utilize anisotropic media (a tensor $\Delta$) so that eq. (4.1) is satisfied only for one orientation of the degenerate cladding fundamental modes.

(iii) Use an asymmetrical cladding so that the cladding fundamental mode is non-degenerate.
(iv) Use a symmetrical cladding with a doubly degenerate fundamental mode, but one in which $|D_e|$ is different for the two polarizations (due to cladding inhomogeneity) so that eq. (4.1) can be satisfied for one polarization but not the other.

Almost all previous single-polarization waveguide designs seem to fall into strategies (i) [29, 42, 47, 51, 91, 99, 111, 112, 114, 123, 137, 138, 165, 175, 185, 187, 208, 212] and (ii) [30, 31, 43, 161, 181, 212], whereas strategies (iii) and (iv) are the only ones that have no long-wavelength cutoff for single-polarization guidance using isotropic materials. Strategy (iii) was previously discussed in a work by Steel and Osgood [183], although they did not remark upon the the cutoff-free nature of the SPSM region (which is difficult to establish numerically in the absence of an analytical theorem like the one here [109, 203]). We discuss each of these strategies, in turn, below, and give examples embodying strategies (iii) and (iv).

4.2.4 Strategy (i)

In this category, we include all SPSM structures that violate the conditions of our theorem entirely, including waveguides that do not rely upon index-guiding. Perhaps the most common such technique to achieve an SPSM fiber is to design a waveguide in which both polarizations have cutoffs, albeit at different frequencies because of some asymmetry. In order to do this, one must violate the conditions of our theorem, which otherwise would guarantee that a guided mode exists. One way to do this is to use a non-periodic cladding, such as an asymmetrical substrate (e.g. an silicon-on-insulator waveguide with air above), which leads to a long-wavelength cutoff for all guided modes of a waveguide [28, 81]. With a periodic (or homogeneous) cladding, our theorem implies that a waveguide in which all modes are cut off must have a $\Delta \varepsilon$ that is negative in some regions (since $\Delta \varepsilon \geq 0$ yields a cutoff-free guided mode). To accomplish this, the oldest technique is a W-profile fiber, in which a higher-index core is surrounded by a depressed-index inner cladding, leading to a cutoff [92] and to an SPSM bandwidth if some asymmetry is introduced [112, 123, 175]. Other geometries
include side-pit or bow-tie fibers, in which the depressed-index regions are located asymmetrically on two sides of the core (instead of surrounding it as in W-profile fibers) [111, 137, 138, 187]. More recently, photonic-crystal holey fibers have used combinations of removed or shrunk holes ($\Delta\varepsilon > 0$) and enlarged holes ($\Delta\varepsilon < 0$) to cut off both guided modes [29, 42, 47, 51, 91, 99, 114, 165, 185, 208]. Fibers that guide light by a photonic bandgap [15, 87, 162, 213], e.g. in a hollow core, also have long-wavelength cutoffs of the gap-guided modes for all polarizations—in the long-wavelength limit, any periodic dielectric structure can be described by an effective homogeneous material [178] and hence has no bandgap. (Gap-guided modes fall outside the confines of our theorem because they do not lie below the cladding light cone.)

However, there is one notable example of a waveguide that violates the conditions of our theorem and yet has a cutoff-free SPSM region: a coaxial metallic waveguide with its non-degenerate cutoff-free TEM mode [197]. This case lies outside the conditions of the theorem because it requires metallic ($\varepsilon < 0$) materials and does not operate by index-guiding. Related single-polarization modes can also be confined by photonic bandgaps in symmetrical coaxial structures [82], but these modes have a long-wavelength cutoff (as for all bandgap guidance, as explained above).

### 4.2.5 Strategy (ii)

Another strategy for SPSM fibers is to use an anisotropic $\varepsilon$. The most obvious technique would be to use an $\Delta\varepsilon$ that is positive for one polarization and negative (or zero) for the other, which therefore will guide only one polarization (which is cutoff-free). In the context of our theorem, this strategy appears as an anisotropic (tensor) $\Delta$, such that eq. (4.1) is satisfied for one degenerate fundamental cladding mode $D_c^{(1)}$ but not for the orthogonal fundamental mode. Experimentally, this has been achieved/proposed using stress birefringence [30, 31, 43, 161, 181] or by liquid crystal filling the core of a holey fiber [212]. Note that by varying various parameters, the design in Ref. 212 can have a cutoff for both guided modes (strategy (i)).
Figure 4-8: Dispersion relations of structures with an asymmetric cladding with no two-dimensional irreducible presentation. In both cases, the fundamental polarization is rigorously cutoff-free, with a single-polarization region below the second-mode cutoff at $\beta = 0.82$ and $\beta = 0.5$ respectively. Here, we plot the mode frequency $\omega$ as $\omega_c - \omega$, where $\omega_c$ is the light-line frequency—this difference is positive for a guided mode.

4.2.6 Strategy (iii)

In order to obtain a cutoff-free SPSM region without using anisotropic materials, perhaps the simplest strategy is to use a periodic cladding with an asymmetrical unit cell so that the fundamental cladding mode is nondegenerate. For example, one could use a triangular or square lattice of elliptical holes [29, 94, 115, 183], or a rectangular lattice of circular holes [208], or many other possibilities. Then, filling in a hole (or some similar $\Delta \varepsilon \geq 0$ core), as in the structure of Ref. 183, guarantees at least one cutoff-free guided mode by our theorem, but there is no such expectation of a second cutoff-free mode.

In fact, we conjecture that the second guided mode will always have a long-wavelength cutoff in the case where the fundamental cladding mode is nondegenerate (that is, that this is a sufficient condition for SPSM guidance). This prediction is borne out by numerical calculations for a variety of structures, such as the triangular
lattice of elliptical holes or rectangular lattice of cylindrical holes, in both cases with
a missing-hole core, shown in Fig. 4-8. Ref. 183 pointed out the existence of an SPSM
region for a triangular lattice of elliptical holes, but did not note the lack of a cutoff
(which is difficult to establish numerically [109, 203]). Our theorem establishes the
lack of a cutoff for the fundamental mode, and provides a necessary condition for the
second mode to have a cutoff (i.e., an SPSM region), but not a sufficient condition
for SPSM. An intuitive argument for why the second mode should have a cutoff is
that, in the long-wavelength regime, the guided modes asymptotically approach a
 corresponding extended mode of the cladding, but the second guided mode in this
case approaches a cladding mode that is above the nondegenerate cladding light line
(and hence is not guided below some cutoff where it crosses the light line).

Several authors have suggested SPSM waveguides based on a combination of non-
degenerate claddings (e.g. elliptical holes) and cores with both positive and nega-
tive $\Delta\varepsilon$ to cut off both polarizations [29, 208], in some sense combining strategies
(i) and (iii). Not apparent in that work is the fact that the negative $\Delta\varepsilon$ regions
(enlarged holes) were superfluous, and an asymmetrical cladding alone is sufficient
to attain SPSM. Other authors have used elliptical holes or rectangular lattices to
achieve birefringence rather than SPSM [125, 199].

4.2.7 Strategy (iv)

A fourth strategy is suggested by the fact that the cladding fundamental-mode field
pattern $|\mathbf{D}_c^{(1,2)}|$ is neither uniform in space nor symmetrical even for a symmetrical
cladding with a doubly degenerate light line, as long as the cladding is inhomogeneous.
This is shown in Fig. 4-9, for the doubly degenerate fundamental modes of a triangular
lattice of air holes in silica. Because of this, it is possible to arrange a core composed
of positive and negative $\Delta\varepsilon$ so that eq. (4.1) is true for one fundamental cladding
mode but not the other. If we do this in the long-wavelength limit, then we will
again obtain a cutoff-free SPSM region. An example of this is shown in the inset of
Fig. 4-10: we form a core by a small cylinder of $\Delta = -0.18$ ($\Delta\varepsilon > 0$) in a region
where $|\mathbf{D}_c^{(1)}|$ is peaked (and where $|\mathbf{D}_c^{(2)}|$ is small) and a small cylinder of $\Delta = +0.18$
Figure 4-9: $|\mathbf{D}_c^{(1,2)}|^2$ field patterns of the two degenerate fundamental space-filling modes of the cladding of the structure in Fig. 4-10. We can utilize the asymmetry of the degenerate cladding mode and design an asymmetric core such that eq. (4.1) is satisfied for one cladding mode but not the other.

$(\Delta \varepsilon < 0)$ in a region where $|\mathbf{D}_c^{(2)}|$ is peaked (and where $|\mathbf{D}_c^{(1)}|$ is small). This yields a cutoff-free SPSM region shown in Fig. 4-10. This strategy is fundamentally different from the previous three in the sense that it is cutoff-free unlike (i), uses isotropic materials unlike (ii), and uses a symmetrical cladding with a degenerate fundamental mode unlike (iii).

There are several subtleties to this approach. First, there are many choices of linear combinations of the degenerate cladding modes $\mathbf{D}_c^{(1,2)}$, and it is only necessary to find one pair that has an asymmetrical $|\mathbf{D}_c^{(1,2)}|$. In the case of Fig. 4-9, the field patterns were chosen corresponding to two “orthogonal” polarizations, or more technically to be even and odd with respect to orthogonal mirror planes [87]; the fact that the same modes could be combined into “circular” polarizations $\mathbf{D}_c^{(1)} \pm i\mathbf{D}_c^{(2)}$ with identical $|\mathbf{D}_c^{(\pm)}|$ patterns is irrelevant because the theorem for two guided modes required eq. (4.1) to be satisfied for all linear combinations. Another difficulty arises because the condition for two guided modes is only a sufficient condition, not a necessary one—as remarked upon in our previous work [109], it becomes overly strong when large $\Delta \varepsilon$ regions are present, in which case we suspect that a weaker (necessary) condition would involve the polarizability of the defects as in our previous work on perturbation theory [90]. Because of this, when $\Delta \varepsilon$ becomes large (e.g. if the defects are created by enlarging and/or shrinking air holes), violating eq. (4.1) for one of the
Figure 4-10: Dispersion relation of a structure with an asymmetrical core in a symmetrical cladding of circular air holes (radius 0.47a in a hexagonal lattice with n = 1.87). The core is formed by two small cylinders of $\Delta = \pm 0.18$, respectively, shown in the inset as light and dark circles in the veins between two pairs of air holes. Here, we plot the mode frequency $\omega$ as $\omega_c - \omega$, where $\omega_c$ is the light-line frequency—this difference is positive for a guided mode.

fundamental modes is not enough to predict whether the second guided mode has a cutoff, and numerical calculations are required.

4.2.8 Summarizing remarks

We have demonstrated the necessary conditions to obtain single-polarization single-mode (SPSM) waveguides, by generalizing previous results to show the sufficient conditions for the existence of two index-guided modes for general microstructured dielectric fibers. According to these conditions, we have categorized single-polarization waveguides into four groups: (i) those that violate the conditions of our theorem entirely, typically resulting in a cutoff for both polarizations; (ii) those that employ anisotropic materials to guide one polarization and not the other; (iii) those using an asymmetrical cladding structure (e.g. an asymmetrical photonic crystal) that does not have a doubly degenerate light-line mode; and (iv) those with a symmetrical periodic cladding that exploit the asymmetry of the light-line’s two polarizations to guide
one polarization but not the other. We have shown that the latter two categories can guarantee cutoff-free single-polarization regions with isotropic materials without relying on birefringent materials. They require an inhomogeneous fiber cladding, such as in a photonic-crystal fiber (a periodic cladding), as opposed to traditional dielectric waveguides surrounded by asymptotically homogeneous cladding materials.

Some questions remain as to what the necessary and sufficient conditions for SPSM fiber designs are. For example, does a nondegenerate light line guarantee that the second mode necessarily have a cutoff? We conjecture that this is the case, but have only an intuitive argument: since the fundamental cladding modes are nondegenerate, and the guided modes approach the cladding modes as $\beta \to 0$, we expect the second guided mode to asymptotically approach the second cladding mode for small $\beta$, and hence it should intersect the light line as a nonzero frequency.

### 4.3 Sufficient conditions for two-dimensional localization by arbitrarily weak defects in periodic potentials with bandgaps for the Schrodinger operator

In this work, led by my collaborator A. Parzgnat and published in Ref. 141, we extend the ideas in the earlier sections to prove, via an elementary variational method, 1D and 2D localization within the bandgaps of a periodic Schrödinger operator for any mostly negative or mostly positive defect potential, $V$, whose depth is not too great compared to the size of the gap. In a similar way, we also prove sufficient conditions for 1D and 2D localization below the ground state of such an operator. Furthermore, we extend our results to 1D and 2D localization in $d$ dimensions; for example, by a linear or planar defect in a 3D crystal. For the case of $D$-fold degenerate band edges, we also give sufficient conditions for localization of up to $D$ states.

This work was initially motivated by the desire to prove a bandgap guidance result.
for small defects in microstructured waveguides—the large defect case has been proven in Ref. 100. Just as we did for the index-guiding case, we attempted to start with the analogous quantum result: confinement in crystals with electronic bandgaps using defects in the crystal. However, such result did not exist — no one had proved the requisite confinement conditions for in more than one dimension even for quantum mechanics. Both as a prerequisite for the electromagnetic case, and because quantum confinement by bandgaps is of fundamental interest in its own right for solid-state physics [8], we set out to prove conditions for quantum bandgap confinement.

Localization by impurities in periodic potentials with spectral gaps (bandgaps) is a central topic in solid-state physics and semiconductor devices, [8] and it has direct analogues for other propagating-wave systems, such as for photonic crystals in electromagnetism. [87] We prove that, in one and two dimensions (1D and 2D), localized solutions must arise in the gaps of a periodic Schrödinger operator for any “mostly” negative or mostly positive defect potential whose depth is not too great compared to the size of the gap. To our knowledge, this is the first rigorous sufficient condition of this sort in 2D, aside from informal arguments based on effective-mass free-electron models close to quadratic gap edges, [130] extending an earlier theorem for 1D localization in gaps, [150] and is quite different from the many rigorous asymptotic gap-localization results in the limit of very strong defect potentials. [38,61,72,80,149,164] In addition to localization in gaps, we also prove 1D and 2D localization below the ground state of a periodic potential for any mostly negative defect potential, extending earlier known results for localization in vacuum for any mostly negative potential [41,174,205], localization in the periodic case but for a strictly non-positive defect potential, [53,79] and 1D localization for mostly negative defects. [150] Furthermore, we extend our results to 1D and 2D localization in d dimensions; for example, establishing localization for a linear or planar defect in a 3D crystal. For the case of D-fold degenerate band edges, we show localization of D bound states for definite-sign defect potentials, and more generally relate the number of localized modes to the signs of the eigenvalues of a $D \times D$ matrix. Our proofs rely only on elementary variational eigenvalue bounds, generalizing an approach developed in Ref. 205.
One-dimensional localization in vacuum by an arbitrary attractive potential is easy to prove by the variational method, at the level of an undergraduate homework problem, [104] while a minimum non-zero depth for a potential well is required for localization in vacuum in three dimensions. [22] The 2D case is more challenging to analyze. The first proof of 2D localization in vacuum by an arbitrary attractive potential was presented in 1976 by Simon, [174] using more sophisticated techniques that also lead to asymptotic properties of the bound states. An elementary variational proof in vacuum was proposed by Picq [10,148] (and was adapted to Maxwell’s equations in optical fibers by Bamberger and Bonnet [10]), while a different variational proof was independently developed by Yang and de Llano. [205] An informal asymptotic argument utilizing properties of the vacuum Green’s function was presented by Economou. [41] On the other hand, in the case of periodic potentials, rigorous results for the existence of bound states from weak defect potentials $V$ are more limited. Frank et al. [53] analyzed the case of potentials $V \leq 0$ localizing at energies below the ground state of a 2D periodic Schrödinger operator; they not only proved that a localized state exists, but also bounded its energy in terms of a related vacuum localization problem. Here, we use a different technique, based on the variational method of Ref. 205, to prove existence of localized modes in 1D and 2D for any indefinite-sign but “mostly” negative defect potential $V$. This is closely related to our generalization of Ref. 205 to index guiding in the periodic Maxwell’s equations. [109] (Indefinite-sign localization was also considered for discrete Schrödinger operators. [37]) As for localization in arbitrary gaps, however, we are not aware of published rigorous results in 2D that are valid for weak $V$. Prodan [150] proved that arbitrarily weak defects localize states in 1D gaps, using an asymptotic Birman-Schwinger technique similar to Ref. 174, imposing a mostly negative/positive condition on the defect potential identical to the one we use below; Prodan’s result also applies to localization below the ground state of a periodic 1D potential. Various authors have shown that for strong defect potentials, those of the form $\lambda V$ where $\lambda \to \infty$, there exists a bound on the number of eigenvalues crossing the gap. [38,61,72,80,164] Localization has also been proved in the limit of high-order gaps in 1D. [62] Another common, albeit somewhat
informal, approach to gap localization is to consider localization for energies close to a non-degenerate quadratic band edge, making an effective-mass approximation and then quoting the results for vacuum. [130] Our proof of localization in gaps is non-asymptotic, does not assume a particular form of the band edge, and is an extension of the elementary variational technique of Ref. 205 for localization in vacuum. The trick behind the variational proof is to take the mid-gap energy, $E_g$, of the perturbed Schrödinger operator, $H$, and transform the question of energies near $E_g$ into an extremal eigenvalue problem. There are two typical ways to do this. One is to consider $(H - E_g)^{-1}$, which seems closely related to the Green's function method of Ref. 41 and to the Birmann–Schwinger condition, [73] but such an operator is hard to evaluate explicitly and mainly lends itself to asymptotic analyses. Another method is to consider $(H - E_g)^2$, recently used for another variational-type localization proof by Ref. 100, and it is this method that we adopt here. The same techniques are used in numerical methods to iteratively compute eigenvalues in the interior of the spectrum of a large matrix, where $(H - E_g)^{-1}$ corresponds to well-known shift-and-invert methods, [9] and where $(H - E_g)^2$ has also been used (but is computationally suboptimal because it squares the condition number). [89,198] Other possible techniques [62,80,202] have been suggested to us [151] for proving such a theorem, but we are not aware of any published results for this problem other than the 1D result of Ref. 150. Localization by weak defects is also related to self-focusing of solitons by nonlinearities, which was recently considered for spectral gaps in periodic potentials. [84]

The contents of the individual sections are summarized as follows. Sec. 4.3.1 provides a simple variational proof of the fact that any arbitrary mostly negative and sufficiently localized defect induces at least one bound state below the infimum of the spectrum of a 2D periodic Schrödinger operator. The 1D case is proved in a similar fashion. Sec. 4.3.2 gives a generalization of that result by allowing the unperturbed Hamiltonian to be periodic in $d$ dimensions and our defect potential to localize in two (or one) dimensions, but be periodic (with the same periodicity as the unperturbed potential) in the other $d - 2$ (or $d - 1$) dimensions. Sec. 4.3.3 presents our main results: it gives a sufficient condition for the existence of a bound state in
the spectral gap of a 2D periodic Schrödinger operator. The results from Sec. 4.3.2 can be applied to this case as well to allow periodicity in any arbitrary extra number of dimensions (although the solution is only localized in two of these dimensions). The case of bound states in a gap confined along one dimension is proved in a similar way. Sec. 4.3.4 describes the case of degenerate band edges as well as some other possible generalizations. Sec. 4.3.5 closes with some concluding remarks and possible future directions.

4.3.1 Bound States Below the Ground State of a Periodic Potential

Notation: In this section, unless otherwise stated, the symbol \( \int f \) will stand for the integral over all of \( \mathbb{R}^2 \) of the real-valued function \( f \).

The proof of the following will be a little simpler than the one in Sec. 4.3.3. However, the ideas used here are almost the same as those of the proof in Sec. 4.3.3, so it is hoped that after going through this proof, the reader will easily follow the latter. Note that the theorem in this section has also been proved by other methods, but only for defect potentials that are strictly nonpositive. [53,79] This theorem will be slightly generalized to allow for a defect potential that is localized in two dimensions, but has an arbitrary periodicity in all other dimensions, in Sec. 4.3.2.

Problem statement

Suppose we start with an unperturbed Hamiltonian,

\[
H_0 = -\nabla^2 + V_0, \tag{4.25}
\]

where \( V_0 \) is a periodic potential (possible generalization to non-periodic potentials is discussed in Sec. 4.3.4), which has a minimum energy eigenvalue \( E_0 \) with at least one (degeneracy will be explored in Sec. 4.3.4) corresponding "generalized" eigenfunction \( \varphi_0 \) of the Bloch form: [8] a periodic function with the same periodicity as \( V_0 \) multiplied by \( e^{i\mathbf{k}\cdot\mathbf{x}} \), giving a bounded \( |\varphi_0| \). We introduce a localized, indefinite (varying sign)
Figure 4-11: Example of a periodic potential $V_0$ and defect potential $V$ with the spectrum $\sigma(H_0)$ located at the right. The spectrum of the unperturbed Schrödinger operator has an infimum $E_0$, and may also have a gap in the set $(E_1, E_2)$.

defect, $V$, giving a new Hamiltonian $H = H_0 + V$, satisfying the two conditions

$$\int V|\psi_0|^2 < 0 \quad \text{and} \quad \lim_{r \to \infty} V(r, \theta) = 0.$$  \hspace{1cm} (4.26)

Such $V_0$ and $V$ are shown schematically in Fig. 4-11 along with a typical spectrum showing $E_0$ (and also possibly a gap, which is considered in Sec. 4.3.3). We prove that conditions (4.26) and (4.27) are sufficient to guarantee the existence of a bound state with energy lower than $E_0$. [Strictly speaking, in order for an energy $< E_0$ to be a “bound” state, the potential $V$ must be sufficiently localized so as to not alter the essential spectrum (energies of non-localized modes) of $H_0$; (4.27) does not appear to be strong enough. Weyl’s theorem provides a sufficient condition of relatively compact $V$, such as the Kato class of mostly square-integrable potentials, which seems to include most realistic localized defects. [76,168]] The proof is essentially a generalization of that in Ref. 205.

**Proof of 2D localization**

Recall that the variational principle (or min–max principle) states that the Rayleigh quotient $\langle \psi, H \psi \rangle / \langle \psi, \psi \rangle$, where $\langle \psi, \phi \rangle \equiv \int \psi^* \phi$ denotes the inner product between $\psi$ and $\phi$ (and $||\psi||^2 \text{ denotes } \langle \psi, \psi \rangle$), for any trial function $\psi$ (in the appropriate Sobolev space) is an upper bound for the ground-state eigenvalue of a Hermitian operator $H$. [65,156,171] Therefore, to prove the existence of an eigenvalue less than $E_0$ (and
thus a bound state), it suffices to find a wavefunction $\psi$ such that

$$E[\psi] = \frac{\langle \psi, (H - E_0)\psi \rangle}{\langle \psi, \psi \rangle} < 0.$$  \hspace{1cm} (4.28)

The key point is to find a trial function that will work even for an arbitrarily small defect $V$. Motivated by Ref. 205, we use the following trial function parametrized by a positive number $\alpha$:

$$\psi = \psi_0 \gamma, \quad \text{where} \quad \gamma = e^{-a(1+r)^{\alpha}}.$$  \hspace{1cm} (4.29)

Once the appropriate trial function is selected, the remaining analysis is straightforward in principle—one simply plugs the trial function into $E[\psi]$ and finds an $\alpha > 0$ where it is negative. The easiest way to do this is to take the $\alpha \to 0$ limit of the numerator: if this limit is negative, then there must also exist a small $\alpha > 0$ where it is negative. This process, which requires some care in taking the limits (limits and integration cannot be interchanged in general), is carried out as follows.

Note that $\gamma$ is already in polar coordinates and that $\psi$ is normalizable for all such $\alpha$ since $\psi_0$ is bounded. This trial function has the key physically motivated property that the limit of no localization, i.e. $\alpha \to 0$, gives the unperturbed ground state $\psi_0$.

We write down the first two derivatives of $\gamma$ for future reference:

$$\gamma' \equiv \frac{\partial \gamma}{\partial r} = \hat{r} \cdot \nabla \gamma = -\alpha (1 + r)^{\alpha-1} \gamma;$$  \hspace{1cm} (4.30)

$$\gamma'' \equiv \frac{\partial^2 \gamma}{\partial r^2} = \alpha (1 + r)^{\alpha-2} [\alpha (1 + r)^{\alpha} - \alpha + 1] \gamma.$$  \hspace{1cm} (4.31)

When $H - E_0$ acts only on $\psi_0$ in $E[\psi]$, the result is zero. The remaining terms in the Rayleigh-quotient numerator, denoted by $U[\psi]$, come from $V$ and derivatives of $\gamma$. After some algebraic simplifications, $U[\psi]$ is given by (see Appendix 4B)

$$U[\psi] = \langle \psi, (H - E_0)\psi \rangle$$

$$= \int V|\psi|^2 + \int |\psi_0|^2 \left[ \frac{1}{2} \nabla^2 (\gamma^2) - \gamma \nabla^2 \gamma \right].$$  \hspace{1cm} (4.32)
Using equations (4.30) and (4.31), we obtain

\[ \nabla^2 \gamma = \alpha(1+r)^{\alpha-2} \left[ \alpha(1+r)^\alpha - \alpha - \frac{1}{r} \right] \gamma; \quad (4.33) \]

\[ \nabla^2 (\gamma^2) = 2\alpha(1+r)^{\alpha-2} \left[ 2\alpha(1+r)^\alpha - \alpha - \frac{1}{r} \right] \gamma^2. \quad (4.34) \]

Plugging these two formulas into \( U[\psi] \) results in the concise form:

\[ U[\psi] = \int V|\psi|^2 + \int |\psi_0|^2 \alpha^2 (1+r)^{2\alpha-2} \gamma^2. \quad (4.35) \]

Note that the denominator of \( E[\psi] \) (which is \( ||\psi||^2 \)) is always positive and so does not affect the sign of \( U[\psi] \). We want to show that \( U[\psi] \), and thus \( E[\psi] \), will be negative for some choice of \( \alpha \). This will be done by showing that the term on the right of equation (4.35) tends to zero as \( \alpha \to 0 \), while \( \int V|\psi|^2 \) will be negative in this limit.

Because \( |\psi_0|^2 \) is bounded, we have

\[
\int |\psi_0|^2 \alpha^2 (1+r)^{2\alpha-2} \gamma^2 \\
\leq 2\pi \max\{|\psi_0|^2\} \int_0^{\infty} \alpha^2 (1+r)^{2\alpha-2} \gamma^2 r dr \\
= 2\pi \max\{|\psi_0|^2\} \int_1^{\infty} \alpha^2 u^{2\alpha-2} \gamma^2 (u-1) du \\
\leq 2\pi \max\{|\psi_0|^2\} \int_1^{\infty} \alpha^2 u^{2\alpha-1} \gamma^2 du, \quad (4.36)
\]

where we have made the substitution \( u = 1 + r \) and then bounded the integral again.

Hence, it suffices to show that the latter integral tends to zero. We calculate this integral explicitly via integration by parts:

\[
\int_1^{\infty} \alpha^2 u^{2\alpha-1} \gamma^2 du \\
= -\frac{\alpha}{2} u^\alpha e^{-2u^\alpha} \bigg|_1^{\infty} + \int_1^{\infty} \frac{\alpha^2}{2} u^{\alpha-1} e^{-2u^\alpha} du = \frac{3\alpha}{4e^2}. \quad (4.37)
\]

Taking the limit as \( \alpha \to 0 \) yields zero as claimed above.
The leftover $\int V|\psi|^2$ term can be split into two parts. Let $V = V^+ - V^-$, where $V^+$ and $V^-$ are the positive and negative parts of $V$. Then we have

$$\int |\psi|^2 V = \int |\psi|^2 V^+ - \int |\psi|^2 V^-,$$

(4.38)

where each $|\psi|^2 V^\pm$ is a monotonically increasing function as $\alpha$ decreases. This allows us to use Lebesgue's monotone convergence theorem [160] to interchange the limit with the integration, arriving at

$$\lim_{\alpha \to 0} \int |\psi|^2 V^\pm = \int \lim_{\alpha \to 0} |\psi|^2 V^\pm = e^{-2} \int |\psi_0|^2 V^\pm$$

(4.39)

for each part. Putting all the information together, we have

$$\lim_{\alpha \to 0} \left( \int V|\psi|^2 + \int |\psi_0|^2 \alpha^2 (1 + r)^{2\alpha - 2\gamma^2} \right)$$

$$= e^{-2} \int |\psi_0|^2 V < 0$$

(4.40)

by our main assumption (4.26). Hence, the variational principle says that there exists an eigenvalue below $E_0$ for the system and so the theorem is proved.

**Proof of 1D localization**

The case for 1D localization can be proved in an analogous way, with simpler calculations, by using the trial function $\psi_0 e^{-\alpha x^2}$.

A closely related result in 1D was presented by Prodan: [150] for any defect potential $V$ satisfying (4.26), and for any energy $E < E_0$, Prodan showed that there was some scaling $\lambda V$ with $\lambda > 0$ such that a bound state with energy $E$ exists. Furthermore, the limit $E \to E_0$ was shown to correspond to $\lambda \to 0$, so that an arbitrarily weak potential satisfying (4.26) must localize a state.
4.3.2 2D Localization in \( d \) Dimensions

We would like to extend these results to an unperturbed Hamiltonian \( H_0 = -\nabla^2 + V_0 \) that is periodic in \( d \) dimensions and where the defect potential \( V \) is localized along one or two dimensions and is periodic in the other dimensions. A physical example of 2D localization would be a linear defect or "quantum wire" in a 3D crystal, localizing a wavefunction to propagate along the line, whereas an example of 1D localization in 3D would be a planar defect.

Periodicity of \( V_0 \) and \( V \)

In this case, \( V_0 \) is a periodic potential in \( d \) dimensions, while \( V \) is periodic only in \( d-2 \) dimensions but localized in the other two. It is convenient to separate the periodic and nonperiodic coordinates of \( V \) by writing \( V \) as \( V(r, \theta, z) \), where \( z \in \mathbb{R}^{d-2} \), which is periodic in \( z \) with some lattice vectors. The first two coordinates are in polar form for convenience in defining what we mean by "localization," which occurs in \( r \) only. \( V_0 \), on the other hand, is periodic in all dimensions, but for convenience, we also write it as \( V_0(r, \theta, z) \). A schematic 2D example of such \( V \) and \( V_0 \), where \( V \) is localized in only one dimension and periodic in one other, is shown in Fig. 4-12. Note that it is irrelevant in our proof whether \( V_0 \) is periodic in any \((r, \theta)\) plane, which only occurs if \((r, \theta)\) corresponds to a lattice plane [8] of \( V_0 \) (such an orthogonal supercell exists only under certain conditions on the lattice vectors [23]).

The corresponding Laplacian for these coordinates is:

\[
\nabla^2 = \nabla^2_{r, \theta} + \nabla^2_z = \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \right) + \sum_{j=3}^{d} \frac{\partial^2}{\partial x_j^2} . \tag{4.41}
\]

In this section and the next, the symbol \( \int f \) will be interpreted as

\[
\int f \equiv \int_0^\infty r \, dr \int_0^{2\pi} d\theta \int_\Omega d^{d-2}z \, f(r, \theta, z), \tag{4.42}
\]

where \( \Omega \) is the primitive cell in \( z \).
Figure 4-12: Linear defect for a periodic lattice (red circles) in two dimensions is created by adding a defect potential (blue circles) that is periodic along the $z$ direction, commensurate with the periodicity of the underlying lattice. This will localize a state with respect to the perpendicular directions, denoted $r$. 
Generalized localization below ground state

Due to the periodicity of the potentials, we apply Bloch’s theorem to reduce this problem to a unit cell in \( z \), in which case a “localized” mode is a point eigenvalue as in the previous section, and we can prove localization by an identical variational approach.

In particular, all eigensolutions can be chosen in the Bloch form \( \psi_0 = \psi_0^k(r, \theta, z)e^{ikz} \), where \( \psi_0^k \) is periodic in \( z \) with the same periodicity as \( V \) (and \( V_0 \)) and \( k \) is some Bloch wavevector. [8] Substituting this into \( H_0\psi = E\psi \), one obtains the “reduced” Hamiltonian

\[
H_0^k = -\nabla^2 - 2ik \cdot \nabla_z + k^2 + V_0,
\]

whose eigenvalues \( E(k) \) are the \( k \)-dependent band structures. The domain is now only the primitive cell in \( z \) with periodic boundary conditions. For each \( k \), there is a minimum energy, \( E_0(k) \), associated with each reduced Hamiltonian \( H_0^k \), i.e. \( H_0^k\psi_0^k = E_0(k)\psi_0^k \) for some Bloch wavefunction \( \psi_0^k \). \( (\psi_0^k e^{ikz} \) is merely one of the Bloch wavefunctions for the underlying potential \( V_0 \) such that the projection of the original \( d \)-dimensional Bloch wavevector onto the \( z \) dimensions gives \( k \). Therefore, \( |\psi_0^k| \) is bounded.) The claim we wish to prove is that the above conditions (just as in Sec. 4.3.1) guarantee the existence of a bound state with energy below \( E_0(k) \) for each \( k \). Moreover, the previous theorem of Sec. 4.3.1 becomes merely the special case when \( k = 0 \) and there are no extra dimensions of periodicity.

Proof of 2D localization in \( d \) dimensions

The proof follows the same outline as in Sec. 4.3.1 (just replace \( \psi_0 \) with \( \psi_0^k \)). There are only two small differences. \( H_0^k \) in (4.43) has the additional terms \( 2ik \cdot \nabla_z \) and \( k^2 \), but \( \nabla_z \gamma = 0 \) so this additional term only acts on \( \psi_0^k \), and is part of the \( (H_0 - E_0)\psi_0^k = 0 \) cancellation as before in (4.32). The second difference is that these integrals are over \( \mathbb{R}^2 \times \mathbb{R}^{d-2} \) (where the part over \( \mathbb{R}^{d-2} \) is actually just over a primitive cell), instead of over \( \mathbb{R}^2 \). This simply means that, in (4.36), instead of factoring out \( \max\{|\psi_0^k|^2| \) in the bound, we factor out \( \max\{|\psi_0^k|^2| \) multiplied by the volume of the primitive cell.
Proof of 1D localization

The analysis is the same except we now have $V_0 = V_0(x, z)$ and $\psi = \psi_0^k e^{ikz} e^{-\alpha z^2}$. The proof proceeds with straightforward application of our proof approach, and will not be presented here.

4.3.3 Bound States Within a Bandgap

Now, we suppose that there is a gap in the spectrum of $H_0^k$ (at a particular $k$ in $d$ dimensions) from $E_1$ up to $E_2$ (with corresponding band edge Bloch wavefunctions $\psi_1^k$ and $\psi_2^k$) as shown in Fig. 4-11, and we prove sufficient conditions for $V$ to localize a state along one or two dimensions with an energy in the gap (with periodicity as defined in the previous section). Intuitively, if $V$ is mostly negative, then a state will be pulled down into the gap from the higher energy edge $E_2$. If it is mostly positive instead, then a state will be pushed up into the gap from the lower energy edge $E_1$. On the other hand, if the potential is too strong, then the band edge state will be pulled/pushed all the way across the gap and will cease to be localized, hinting that we may need some upper bound on the strength of the defect potential even if there is no lower bound. This will be made quantitative in Sec. 4.3.3.

The idea behind the actual proof is to translate it to a simpler problem so that the methods of Sec. 4.3.1 can be used. That is, we must somehow alter the operator $H$ so that we are localizing below the “ground state” of an altered $H_0$ and can use the variational principle. This is achieved by considering $(H - E_g)^2$, where $E_g = (E_2 - E_1)/2$, instead of just $H$, which transforms the spectrum as shown in Fig. 4-13. This idea comes from the localization proofs of Ref. 100 as well as from numerical techniques. [89,198] The trial function is motivated once again by Ref. 205.

Statement of the theorem

For ease of notation, we will omit the $k$ superscripts in this section.
We will prove gap localization under the following conditions. The intuition that $V$ should be mostly negative or positive corresponds to our condition:

$$\int V|\psi_2|^2 < 0 \quad \text{and/or} \quad \int V|\psi_1|^2 > 0. \quad (4.44)$$

The intuition that $V$ cannot be too big corresponds to:

$$2|E_i - E_g| \left| \int V|\psi_i|^2 \right| > \int V^2|\psi_i|^2, \quad (4.45)$$

where $i$ depends on which case of (4.44) was satisfied; that is, from which band edge we are pulling a localized state. [Conditions (4.44)–(4.45) can be merged into a single condition, below, that (4.52) is negative.] We also require that $V$ be sufficiently localized in $r$, corresponding to the condition:

$$\int |V||\psi_i|^2 < \infty \quad \text{and} \quad \int V^2|\psi_i|^2 < \infty. \quad (4.46)$$
These conditions are sufficient to guarantee a bound state in the gap for the perturbed Hamiltonian $H = H_0 + V$, i.e. a localized state in the $(r, \theta)$ dimensions.

**Proof of 2D localization**

Considering one band edge at a time, we will prove localization of a bound state “pulled” from the band edge $E_i$ for $i = 1, 2$. The proof will be split up into several steps to make it easier to follow. The method employed is the same as that in Sec. 4.3.1.

The variational principle in this problem can be used after shifting the center of the gap to the zero position and squaring the resulting operator thus making it sufficient to find a normalizable trial function $\psi$ such that

\[
\frac{\langle \psi, (H - E_g)^2 \psi \rangle}{\langle \psi, \psi \rangle} < (E_i - E_g)^2 \equiv (\Delta E)^2
\]

or equivalently,

\[
\| (H - E_g) \psi \|^2 - (\Delta E)^2 \| \psi \|^2 < 0. \tag{4.48}
\]

Consider the trial function $\psi = \gamma \psi_i$, where $\gamma = \exp\{- (1 + r)^\alpha\}$ as before. Similar to Sec. 4.3.1, we will show that this $\psi$ will satisfy condition (4.48) for some small $\alpha$ providing conditions (4.44)-(4.46) are also satisfied.

After some algebraic manipulation and using the fact that $H_0 \psi_i = E_i \psi_i$, the left-hand side of (4.48) becomes (as shown in more detail in Appendix 4B)

\[
\| (H - E_g) \psi \|^2 - (\Delta E)^2 \| \psi \|^2 =
\]

\[
(\Delta E) \int |\psi_i|^2 \left[ \nabla^2 (\gamma^2) - 2 \gamma \nabla^2 \gamma \right] \tag{4.49}
\]

\[
+ 2(\Delta E) \int V |\psi|^2 + \| V \psi \|^2
\]

\[
- \int V \left[ (\nabla |\psi_i|^2 \cdot \nabla (\gamma^2) - 2|\psi_i|^2 \gamma \nabla^2 \gamma \right]
\]

\[
+ 4 \| \nabla \psi_i \cdot \nabla \gamma \|^2 + \| \psi_i \nabla^2 \gamma \|^2
\]

\[
+ 2 \int \nabla^2 \gamma \nabla |\psi_i|^2 \cdot \nabla \gamma. \tag{4.51}
\]

\[138\]
It is a bit cumbersome, but we can separate the integrals into four main groups to avoid calculating each one individually.

The first group consists of (4.49), but we have already shown that this integral tends to zero as $\alpha \to 0$ in Sec. 4.3.1—see equations (4.36) and (4.37).

The second group consists of all the integrals which involve $V$. These are all contained in (4.50). Taking the limit as $\alpha \to 0$ is allowed to pass through the integrals because everything is bounded by either a constant times $V$ or a constant times $V^2$, and our assumption (4.46) allows us to use Lebesgue's dominated convergence theorem [160] to commute the limits with integration. The limit of these integrals as $\alpha \to 0$ is

$$e^{-2} \int V^2 |\psi_i|^2 + 2(E_i - E_g)e^{-2} \int V|\psi_i|^2,$$

(4.52)

where the rightmost integrand of (4.50) vanishes for $\alpha \to 0$ because differentiating $\gamma$ results in at least one $\alpha$ factor. Equation (4.52) is strictly negative under conditions (4.44) and (4.45). Namely, the $V^2$ term is smaller than the $V$ term by (4.45), and (4.44) implies that the $(E_i - E_g)V|\psi_i|^2$ integral is negative for either $i = 1$ or $i = 2$.

We now move on to the final terms: everything in (4.51). We wish to show that they all tend to zero as $\alpha \to 0$, and we can do this easily by concentrating on the term that decays the most slowly with respect to $r$, so that all the other terms which decay faster clearly go to zero as well (provided that the terms have the same or higher order for the $\alpha$ factor in front). The three integrals of (4.51), dropping bounded terms such as $|\psi_i|^2$, are [from left to right in (4.51)]:

$$(\nabla \gamma)^2 = \alpha^2 (1 + r)^{2\alpha - 2} \gamma^2,$$

(4.53)

$$(\nabla^2 \gamma)^2 = \alpha^2 (1 + r)^{2\alpha - 4} \left[ \alpha (1 + r)^{\alpha} - \alpha - \frac{1}{r} \right]^2 \gamma^2,$$

(4.54)

$$\nabla^2 \gamma \nabla \gamma = \alpha^2 (1 + r)^{2\alpha - 3} \left[ \alpha (1 + r)^{\alpha} - \alpha - \frac{1}{r} \right] \gamma^2.$$

(4.55)

Each has at least an $\alpha^2$ factor in front. Upon inspection, we find that the most slowly decaying term out of these three is the $(\nabla \gamma)^2$ term, which goes as $1/r^2$ in the limit.
of $\alpha \to 0$ and its limit is

$$\lim_{\alpha \to 0} \int_0^\infty \alpha^2 (1 + r)^{2\alpha - 2} r \, dr \to 0,$$

as was already shown in (4.36) and (4.37). Since (4.53) dominates (4.51), the other terms are all asymptotically bounded by some constant times this integral and hence must also have integral zero in the limit as $\alpha \to 0$.

What has been shown is that every term from the left-hand side of (4.48) vanishes except for the one term (4.52), which is negative. This establishes the existence of a bound state.

**Proof of 1D localization**

The case for 1D localization can be proved in an analogous way, with simpler calculations, by using the trial function $\psi_0 e^{-\alpha x^2}$ just as before.

A closely related result in 1D was presented by Prodan: [150] for any defect potential $V$ satisfying (4.44), and for any energy $E$ in the gap, Prodan showed that there was some scaling $\lambda V$ with $\lambda > 0$ such that a bound state with energy $E$ exists. Furthermore, the limit as $E$ approaches the band edge corresponding to (4.44) was shown to correspond to $\lambda \to 0$, so that the limit of an arbitrarily weak potential satisfying (4.44) must localize a state in the gap.

**4.3.4 Some further generalizations**

**Necessity of periodicity?**

In all our derivations, we did not actually explicitly use the fact that $V_0$ was periodic in the dimensions where localization would take place. All we used were a few of the properties of periodic potentials. These are:

The energies are bounded from below.

There may be a finite gap inside the continuous spectrum.
The generalized eigenfunctions corresponding to the infimum/gap-edge energies are bounded (and their derivatives are bounded).

For gap localization, we also assumed that the squared operator was well-defined, making application of this theorem to delta-function potentials (Kronig–Penney models) appear problematic, although it is possible that the difficulty is surmountable with a sufficiently careful limiting process. (In physical contexts, the difference between a theoretical infinite-depth $V_0$ and a finite-depth approximation seems scarcely relevant.) Also, we assumed coinciding essential spectra for $H_0$ and $H$ in order to utilize the variational principle. This means that there are some restrictions on how large of a perturbation $V$ can be. However, Weyl’s theorem states one sufficient condition, [76,168] which appears to be satisfied for most physically interesting $V$’s; see also the comments after (4.27).

The third assumption listed above may be more challenging to prove for non-periodic potentials. We assumed that the energies at the infimum of the spectrum and/or the edges of spectral gaps correspond to eigenvalues with bounded generalized eigenfunctions ($\psi_0$ or $\psi_1$). (This corresponds to the requirement of a regular ground state in Ref. 53.) For periodic potentials, the existence of a band-edge solution for $V_0$ follows from the well-known continuity of the band diagram as a function of the Bloch wavevector $k$. For non-periodic potentials $V_0$, however, this is not necessarily true. For example, for the 1D half-well potential $V_0(x) = \infty$ for $x < 0$ and $= 0$ for $x > 0$, the eigenfunctions $\sin(\kappa x)$ do not have a nonzero infimum-energy solution for $\kappa \to 0$, and correspondingly it is well known that any perturbation $V$ must exceed some threshold depth before a bound state appears in that case—this is mathematically equivalent to the appearance of an odd bound-state solution $\psi(-x) = -\psi(x)$ for $V_0 = 0$ and an even perturbation $V(-x) = V(x)$, which requires a threshold depth since the lowest-energy bound state in that case is even. It is not clear to us under what conditions the requisite infimum/gap-edge solutions exist for more general potentials, such as quasiperiodic potentials $V_0$, although some examples are given in Ref. 53.
Degeneracy at the band edges

As mentioned earlier, it could happen that there are multiple (degenerate) linearly independent \( \psi_i \)'s corresponding to a given energy \( E_i \) at an edge of the gap and/or at the infimum of the spectrum. Our proof in the preceding sections is unaffected—there must still be at least one bound state localized by a suitable \( V \), as long as the requisite conditions [(4.26) or (4.44–4.46)] hold for at least one of the degenerate \( \psi_i \) wavefunctions. Intuitively, however, one might expect to be able to prove a stronger theorem in this case—if \( E_i \) is \( D \)-fold degenerate, can one show that \( D \) localized states are formed by a suitable \( V \)?

To prove the existence of more than one localized state, we can employ a generalization of the min–max theorem. For a single localized state, our proof involved the fact that the ground-state eigenvalue of a Hermitian operator \( O \) is bounded above by the Rayleigh quotient \( Q[\psi] = \langle \psi, O\psi \rangle / \langle \psi, \psi \rangle \) for any \( \psi \). The generalization of this fact is that the \( n \)-th eigenvalue \( \lambda_n \) is bounded above by [10]

\[
\lambda_n \leq \sup_{\psi \in S_n} Q[\psi],
\]

where \( S_n \) is any \( n \)-dimensional subspace of the Sobolev space for \( O \). We then wish to show that \( \lambda_n < b \) for some bound \( b \): \( O = H - E_0 \) and \( b = 0 \) for localization below the infimum of the spectrum, or \( O = (H - E_g)^2 \) and \( b = (E_i - E_g)^2 \) for localization in the gap from edge \( i \). This is equivalent to proving that the Hermitian form \( B[\psi, \phi] = \langle \psi, (O - b)\phi \rangle \) is negative-definite for some \( n \)-dimensional subspace \( S_n \) (i.e., \( B[\psi, \psi] < 0 \) for all \( \psi \in S_n \)).

If \( E_i \) is \( D \)-fold degenerate, with degenerate generalized eigenfunctions \( \psi_i^\ell \) for \( \ell = 1, \ldots, D \), then the analogue of our previous approach is to form the trial functions \( \psi^\ell = \gamma \psi_i^\ell \) (whose span is a subspace \( S_D \)), compute the \( D \times D \) matrix \( B_{\ell \ell'} = B[\psi^\ell, \psi^{\ell'}] \), and check whether it is negative definite as \( \alpha \to 0 \). We wish to find the largest subspace \( S_n \) of \( S_D \) for which \( B \) is negative-definite, which corresponds to the number \( n \) of negative eigenvalues of \( B \): this will be the number \( n \) of localized states that are guaranteed by the theorem.
For localization below the infimum of the spectrum by a defect $V$ satisfying (4.27), following exactly the same steps as in Sec. 4.3.2, proving that $B[\psi, \phi]$ is negative-definite in this subspace reduces to a generalization of condition (4.26). Specifically, showing $B[\psi, \psi] < 0$ in the subspace for $\alpha \to 0$ reduces, via (4.40), to showing that $\int V|\psi|^2 < 0$ for every $\psi$ in the subspace. In other words, the Hermitian form $A[\psi, \phi] = \langle \psi, V\phi \rangle$ must be negative-definite in $S_n$. In the $\alpha \to 0$ limit, this corresponds to checking the eigenvalues of the $D \times D$ matrix $A_{\ell \ell'} = A[\psi_\ell^\ell, \psi_{\ell'}^{\ell'}]$; the number of negative eigenvalues of $A$ is precisely the dimension of the largest negative-definite subspace $S_n$, and hence is the number of bound states that are guaranteed to be localized below the ground state of $V_0$. If we happen to have a strictly non-positive $V \leq 0$, then the Hermitian form $A$ is automatically negative-definite and we are guaranteed $D$ localized modes.

For localization in a gap by a defect $V$ satisfying (4.46), pulling states from band-edge $i$, following exactly the same steps as in Sec. 4.3.3, one finds that $B[\psi, \phi]$ being negative-definite reduces to a generalization of condition (4.52): the Hermitian form $G[\psi, \phi] = \langle \psi, [V^2 + 2(E_i - E_g)V]\phi \rangle$ must be negative-definite in $S_n$. As above, this simplifies for $\alpha \to 0$ to counting the number of negative eigenvalues of the $D \times D$ matrix $G_{\ell \ell'} = G[\psi_{\ell}^{\ell'}, \psi_{\ell'}^{\ell'}]$. The number of negative eigenvalues is the number of solutions that are guaranteed to be localized from band-edge $i$. If $V$ has sign everywhere opposite to $E_i - E_g$ and is sufficiently small (to overwhelm the $V^2$ term), then $D$ eigenstates will be localized from this band edge.

This analysis appears to be closely related to the asymptotic technique of Ref. 202, which also relates the number of bound modes to the number of eigenvalues of a given sign of a small matrix, via the Birman-Schwinger principle in the limit of weak perturbations, but that work only explicitly considered localization below the ground state of translation-invariant elliptic and Schrödinger-type unperturbed operators.

### 4.3.5 Summarizing Remarks

Although the existence of localized solutions from defects in periodic potentials and the effective-mass analogy with the vacuum case are well known as a practical com-
putational and experimental matter, it is gratifying to have a general, explicit proof that localization in one and two dimensions occurs in a similar manner to localization in vacuum. A number of directions suggest themselves for future research. Although the simplicity of an elementary proof based on the min-max/variational theorem has its own appeal, the application of more sophisticated methods such as those of Ref. 174 may reveal additional information about the nature of the localized state (such as its asymptotic localization length) that cannot be gleaned from a simple variational analysis. We would also like to transfer these results from the Schrödinger (scalar) picture to the Maxwell (vector) one, in the context of localization in bandgaps of photonic crystals such as photonic-crystal fibers. [87] A similar generalization to electromagnetism was already obtained for localization below the infimum of the spectrum (corresponding to total internal reflection in Maxwell’s equations) for non-periodic [10] and periodic [109] media, and in photonic bandgaps for sufficiently large defects. [100, 124]

For localization in gaps, we should remark that the condition (4.45) on the size of the perturbation $V$ is somewhat unsatisfying. Intuitively, a “small” perturbation $V$ could be one where either $|V|$ is small at every point or where $|V|$ is not small but the support of $V$ is small. The latter case, however, of a large $|V|$ with a small integral, violates our smallness condition (4.45) for a sufficiently large $|V|$ no matter how small the support might be. This does not mean that there are no localized states in that limit—our proof only gives a sufficient condition for localization, not a necessary condition—but it suggests that some reformulation to handle this physically interesting possibility might be desirable.

**Appendix 4A: List of all Rayleigh-quotient terms in Sec. 4.1**

In this appendix, we provide an exhaustive listing of all the terms that appear when the trial function [eq. (4.21)] is substituted into eq. (4.20) (the condition to be satisfied,
a rearrangement of the Rayleigh quotient bound). Since the terms that contain \( \Delta \) [category (i)] were already fully analyzed in Sec. 4.1.3 (since for these terms the limits could be trivially interchanged), we consider only the remaining terms involving \( \varepsilon_c(r) \). More specifically, the only non-trivial term to analyze is the \( \Delta \)-free part of the left-most integral in eq. (4.20):

\[
\int \mathbf{H}^* \cdot (\nabla_\beta \times \varepsilon_c^{-1} \nabla_\beta \times \mathbf{H})
= \int \mathbf{H}^* \cdot (\nabla_\beta \times \varepsilon_c^{-1} \nabla_\beta \times \mathbf{H}_c) + \int \mathbf{H}^* \cdot (\nabla_\beta \times \varepsilon_c^{-1} \nabla_\gamma \times \mathbf{H}_c) \tag{4.58}
+ \int \mathbf{H}^* \cdot (\nabla_\beta \times \varepsilon_c^{-1} \nabla_\beta \times (\nabla_\gamma \times \mathbf{A}_c)) \, .
\]

We have already seen, in eq. (4.23), that the first term breaks down into a term that cancels \( \frac{-\omega_c^2}{c^2} \int \mathbf{H}^* \cdot \mathbf{H} \) in eq. (4.20), via the eigen-equation, and two other terms. Removing the terms canceled by the eigen-equation, and substituting \( -i\varepsilon_c \mathbf{E}_c \) for \( \varepsilon_c^{-1} \nabla_\beta \times \mathbf{H}_c \) (Ampère’s law), we have:

\[
-\frac{\omega_c^2}{c^2} \int \mathbf{H}^* \cdot (\nabla_\gamma \times \mathbf{A}_c) + \int \mathbf{H}^* \cdot [\nabla_\gamma \times (-i \frac{\omega_c}{c} \mathbf{E}_c)]
+ \int \mathbf{H}^* \cdot \nabla_\beta \times \varepsilon_c^{-1} [\nabla_\gamma \times \mathbf{H}_c + \nabla_\beta \times (\nabla_\gamma \times \mathbf{A}_c)]
= -\frac{\omega_c^2}{c^2} \int [\gamma \mathbf{H}_c + \nabla_\gamma \times \mathbf{A}_c]^* \cdot (\nabla_\gamma \times \mathbf{A}_c) - i \frac{\omega_c}{c} \int \gamma \nabla_\gamma \cdot (\mathbf{E}_c \times \mathbf{H}_c^*)
- i \frac{\omega_c}{c} \int (\nabla_\gamma \times \mathbf{A}_c)^* \cdot (\nabla_\gamma \times \mathbf{E}_c) + \int (\gamma \nabla_\beta \times \mathbf{H}_c)^* \cdot \varepsilon_c^{-1} [\nabla_\gamma \times \mathbf{H}_c + \nabla_\beta \times (\nabla_\gamma \times \mathbf{A}_c)]
+ \int (\nabla_\gamma \times \mathbf{H}_c)^* \cdot \varepsilon_c^{-1} [\nabla_\gamma \times \mathbf{H}_c + \nabla_\beta \times (\nabla_\gamma \times \mathbf{A}_c)]
+ \int (\nabla_\beta \times \nabla_\gamma \times \mathbf{A}_c)^* \cdot \varepsilon_c^{-1} [\nabla_\gamma \times \mathbf{H}_c + \nabla_\beta \times (\nabla_\gamma \times \mathbf{A}_c)]
\]
\[ \begin{align*}
&= -\frac{\omega_c^2}{c^2} \int \gamma \mathbf{H}_c^* \cdot (\nabla \times \mathbf{A}_c) - \frac{\omega_c^2}{c^2} \int \|\nabla \times \mathbf{A}_c\|^2 - i\frac{\omega_c}{c} \int \gamma \nabla \cdot \left( \mathbf{E}_c \times \mathbf{H}_c^* \right) \\
&- \frac{i\omega_c}{c} \int (\nabla \times \mathbf{A}_c)^* \cdot (\nabla \times \mathbf{E}_c) + \frac{i\omega_c}{c} \int \gamma \mathbf{E}_c^* \cdot (\nabla \times \mathbf{H}_c) \\
&+ \frac{i\omega_c}{c} \int \gamma (\nabla \times \mathbf{E}_c)^* \cdot (\nabla \times \mathbf{A}_c) + \frac{i\omega_c}{c} \int (\nabla \times \mathbf{E}_c)^* \cdot (\nabla \times \mathbf{A}_c) \\
&+ \int (\nabla \times \mathbf{H}_c)^* \cdot \varepsilon_c^{-1} (\nabla \times \mathbf{H}_c) \\
&+ \left( \int (\nabla \times \mathbf{H}_c)^* \cdot \varepsilon_c^{-1} [\nabla \times (\nabla \times \mathbf{A}_c)] + \text{c.c.} \right) \\
&+ \int (\nabla \times (\nabla \times \mathbf{A}_c))^* \cdot \varepsilon_c^{-1} (\nabla \times (\nabla \times \mathbf{A}_c)) \\
&= -\frac{\omega_c^2}{c^2} \int \gamma \mathbf{H}_c^* \cdot (\nabla \times \mathbf{A}_c) - \frac{\omega_c^2}{c^2} \int \|\nabla \times \mathbf{A}_c\|^2 - 2i\frac{\omega_c}{c} \int \gamma \nabla \cdot \Re \{\mathbf{E}_c \times \mathbf{H}_c^*\} \\
&+ \left( i\frac{\omega_c}{c} \int (\nabla \times \mathbf{A}_c) \cdot (\nabla \times \mathbf{E}_c)^* + \text{c.c.} \right) + \frac{\omega_c^2}{c^2} \int \gamma \mathbf{H}_c^* \cdot (\nabla \times \mathbf{A}_c) \\
&+ \int (\nabla \times \mathbf{H}_c)^* \cdot \varepsilon_c^{-1} (\nabla \times \mathbf{H}_c) + \left( \int (\nabla \times \mathbf{H}_c)^* \cdot \varepsilon_c^{-1} [\nabla \times (\nabla \times \mathbf{A}_c)] + \text{c.c.} \right) \\
&+ \int (\nabla \times (\nabla \times \mathbf{A}_c))^* \cdot \varepsilon_c^{-1} (\nabla \times (\nabla \times \mathbf{A}_c)) \\
&= -\frac{\omega_c^2}{c^2} \int \gamma \mathbf{H}_c^* \cdot (\nabla \times \mathbf{A}_c) - \frac{\omega_c^2}{c^2} \int \|\nabla \times \mathbf{A}_c\|^2 - 2i\frac{\omega_c}{c} \int \gamma \nabla \cdot \Re \{\mathbf{E}_c \times \mathbf{H}_c^*\} \\
&+ \left( i\frac{\omega_c}{c} \int (\nabla \times \mathbf{A}_c) \cdot (\nabla \times \mathbf{E}_c)^* + \text{c.c.} \right) + \frac{\omega_c^2}{c^2} \int \gamma \mathbf{H}_c^* \cdot (\nabla \times \mathbf{A}_c) \\
&+ \int (\nabla \times \mathbf{H}_c)^* \cdot \varepsilon_c^{-1} (\nabla \times \mathbf{H}_c) + \left( \int (\nabla \times \mathbf{H}_c)^* \cdot \varepsilon_c^{-1} [\nabla \times (\nabla \times \mathbf{A}_c)] + \text{c.c.} \right) \\
&+ \int (\nabla \times (\nabla \times \mathbf{A}_c))^* \cdot \varepsilon_c^{-1} (\nabla \times (\nabla \times \mathbf{A}_c)) \\
&= \frac{\omega_c^2}{c^2} \int \gamma \mathbf{H}_c^* \cdot (\nabla \times \mathbf{A}_c)\] \right.
\end{align*} \]

Above, the first "=" step is obtained by substituting the trial function for \(\mathbf{H}\), integrating some of the \(\nabla \times\) operators by parts, and distributing the derivatives of \(\gamma \mathbf{H}_c\) by the product rule. The second step is obtained by using Ampère's law again, combined with integrations by parts and the product rule; "c.c." stands for the complex conjugate of the preceding expression. Continuing, we obtain:

\[ \begin{align*}
&= -\frac{\omega_c^2}{c^2} \int \gamma \mathbf{H}_c^* \cdot (\nabla \times \mathbf{A}_c) - \frac{\omega_c^2}{c^2} \int \|\nabla \times \mathbf{A}_c\|^2 - 2i\frac{\omega_c}{c} \int \gamma \nabla \cdot \Re \{\mathbf{E}_c \times \mathbf{H}_c^*\} \\
&+ \left( \int (\nabla \times \mathbf{H}_c)^* \cdot \varepsilon_c^{-1} (\nabla \times \mathbf{H}_c) + \left( \int (\nabla \times \mathbf{H}_c)^* \cdot \varepsilon_c^{-1} [\nabla \times (\nabla \times \mathbf{A}_c)] + \text{c.c.} \right) \\
&+ \int (\nabla \times (\nabla \times \mathbf{A}_c))^* \cdot \varepsilon_c^{-1} (\nabla \times (\nabla \times \mathbf{A}_c)) \right. \\
&= \frac{\omega_c^2}{c^2} \int \gamma \mathbf{H}_c^* \cdot (\nabla \times \mathbf{A}_c)\] \right.
\end{align*} \]

In obtaining this expression, we have grouped terms into complex-conjugate pairs and used Faraday's law to replace \(\nabla \times \mathbf{E}_c\) with \(i\frac{\omega_c}{c} \mathbf{H}_c\). At this point, we have two \(\frac{\omega_c^2}{c^2} \int \gamma \mathbf{H}_c^* \cdot (\nabla \times \mathbf{A}_c)\) terms that exactly cancel. All of the remaining terms, except for \(-i\frac{\omega_c}{c} \int \gamma \nabla \cdot \Re \{\mathbf{E}_c \times \mathbf{H}_c^*\}\), are multiples of two first or higher derivatives of \(\gamma\), corresponding to category (iv) and (v) terms, which we proved to vanish in Sec. 4.1.3.

The only remaining term is the \(\mathbf{E}_c \times \mathbf{H}_c^*\) term, in category (iii). This term is identically zero (for any \(\alpha \geq 0\)) because it is purely imaginary, whereas all of the
other terms are purely real and the overall expression must be real. More explicitly:

\[
-2i \frac{\omega_c}{c} \int \gamma \nabla \gamma \cdot \Re \{ \mathbf{E}_c \times \mathbf{H}_c^* \} \\
= -2i \frac{\omega_c}{2c} \int \nabla \gamma^2 \cdot \Re \{ \mathbf{E}_c \times \mathbf{H}_c^* \} \\
= -i \frac{\omega_c}{c} \int \nabla \cdot (\gamma^2 \Re \{ \mathbf{E}_c \times \mathbf{H}_c^* \}) + i \frac{\omega_c}{c} \int \gamma^2 \nabla \cdot (\Re \{ \mathbf{E}_c \times \mathbf{H}_c^* \})
\] (4.61)

The first term of the last line is zero by the divergence theorem (transforming it into a surface integral at infinity), since \( \gamma \to 0 \) at infinity. For the second term, the integrand is the divergence of the time-average Poynting vector \( \Re \{ \mathbf{E}_c \times \mathbf{H}_c^* \} \), which equals the time-average rate of change of the energy density [86], which is identically zero for any lossless eigenmode (such as the cladding fundamental mode).

Appendix 4B: Detailed calculations for Sec. 4.3.1 and Sec. 4.3.3

Here we will provide more details for the calculations of Secs. 4.3.1 and 4.3.3. Let \( \psi \) be an eigenstate multiplied by a real function \( \gamma \) whose derivatives decay quickly enough, i.e. \( \psi = \psi_0 \gamma \) where and \( \gamma \) is real (we can think of the example used in this section) and \( \psi_0 \) is bounded and satisfies \( H_0 \psi_0 = E_0 \psi_0 \). We will explore some of the terms in both \( \langle \psi, (H - E_0)\psi \rangle \) and \( \langle (H - E_g)\psi, (H - E_g)\psi \rangle \). Our goals in the above sections were to show that most terms tended to zero. In order for this to be apparent, we had to perform several algebraic manipulations of the integrals that are given here more explicitly.
Calculations for Sec. 4.3.1

We will derive the general formula used in Sec. 4.3.1 first. We have

\[
(H - E_0)\psi = (-\nabla^2 \psi_0 + V_0 \psi_0)\gamma - E_0 \psi_0 \gamma \\
+ V \psi - 2\nabla \psi_0 \cdot \nabla \gamma - \psi_0 \nabla^2 \gamma \\
= V \psi - 2\nabla \psi_0 \cdot \nabla \gamma - \psi_0 \nabla^2 \gamma
\]  
(4.62)

since \((-\nabla^2 + V_0)\psi_0 = E_0 \psi_0\), so that \(U[\psi] = \langle \psi, (H - E_0)\psi \rangle\) is

\[
U[\psi] = \int V|\psi|^2 - 2 \int \gamma \psi_0^* \nabla \psi_0 \cdot \nabla \gamma - \int |\psi_0|^2 \gamma \nabla^2 \gamma.
\]  
(4.63)

Because \(U[\psi]\) must always be real and \(\gamma\) is assumed to be real, the imaginary part of \(\psi_0^* \nabla \psi_0\) must integrate to zero. Therefore, we can replace \(2\psi_0^* \nabla \psi_0\) by \(\psi_0^* \nabla \psi_0 + \psi_0 \nabla \psi_0^*\) in the integrand. We can also use the identity \(\gamma \nabla \gamma = \frac{1}{2} \nabla (\gamma^2)\) so that equation (4.63) becomes

\[
\int V|\psi|^2 - \frac{1}{2} \int \nabla |\psi_0|^2 \cdot \nabla (\gamma^2) - \int |\psi_0|^2 \gamma \nabla^2 \gamma.
\]  
(4.64)

We now rewrite middle term in another manner in order to eliminate the slowly decaying second derivative of \(\gamma\), using integration by parts:

\[
\int \nabla |\psi_0|^2 \cdot \nabla (\gamma^2) = \int \nabla |\psi_0|^2 \nabla (\gamma^2) - \int |\psi_0|^2 \nabla^2 (\gamma^2)
\]  
(4.65)

\[
= - \int |\psi_0|^2 \nabla^2 (\gamma^2),
\]  
(4.66)

where "\(\int_\partial\)" stands for the boundary integral. The boundary integral is zero because the \(\gamma\) term and its first derivative decay fast enough and \(\psi_0\) is bounded. Therefore, all we have to show in Sec. 4.3.1 is that

\[
\int V|\psi|^2 + \frac{1}{2} \int |\psi_0|^2 \nabla^2 (\gamma^2) - \int |\psi_0|^2 \gamma \nabla^2 \gamma < 0
\]  
(4.67)

for some sufficiently small choice of the parameter \(\alpha\).
Calculations for Sec. 4.3.3

We will now derive the general formula used in Sec. 4.3.3. The same assumptions hold as in the previous subsection, but with minor modifications from Sec. 4.3.3, for example $\psi = \psi_i \gamma$ where $i = 1, 2$ signifies the lower or upper edge of the bandgap, respectively. First, we calculate $(H - E_g)\psi$.

\[
(H - E_g)\psi = (\Delta E)\psi + V\psi - 2\nabla \psi_i \cdot \nabla \gamma - \psi_i \nabla^2 \gamma,
\]

where $\Delta E = E_i - E_g$ as in Sec. 4.3.3. Then the generalized equation for $\| (H - E_g)\psi \|^2$ is given by (employing some of the trivial simplifications from the previous section)

\[
(\Delta E)^2 \| \psi \|^2 + 2(\Delta E) \int V|\psi|^2 + \|V\psi\|^2 \\
- \int V\nabla|\psi_i|^2 \cdot \nabla (\gamma^2) - 2 \int V|\psi_i|^2 \gamma \nabla^2 \gamma \\
- 2(\Delta E) \int |\psi_i|^2 \gamma \nabla^2 \gamma \\
+ \|\psi_i \nabla^2 \gamma\|^2 + 2 \int \nabla^2 \gamma \nabla |\psi_i|^2 \cdot \nabla \gamma \\
- (\Delta E) \int \nabla|\psi_i|^2 \cdot \nabla (\gamma^2) + 4\|\nabla \psi_i \cdot \nabla \gamma\|^2.
\]

Notice that the first term in (4.73) is similar to the middle term in (4.64) from the previous subsection, so the same analysis shows that (4.73) becomes

\[
+ (\Delta E) \int |\psi_i|^2 \nabla^2 (\gamma^2) + 4\|\nabla \psi_i \cdot \nabla \gamma\|^2.
\]

In (4.49) of Sec. 4.3.3, this first term of (4.74) is combined with term (4.71). Several of the other terms are rearranged to make the presentation more concise.
Chapter 5

Design of negatively refracting flat lens for visible wavelengths

In this work, we designed a 3D photonic crystal slab structure to exhibit negative refraction (or NIB, negative-index behavior—even though there is no effective index to speak of) at visible wavelengths. As seen in Chapter 1, our goal was to realize negative refraction in visible wavelengths for use as a starting point for progress in, for example, flat-lens imaging and lithography applications. We will explain the physical principles of how our design works, then outline the process of our theoretical design, and finally describe our experimental collaborators’ characterization of the structures that they fabricated.

5.1 Physical principles of operation

To begin with, we review the underlying physical principles governing refraction at the interface between a homogeneous medium and a periodic medium (a photonic crystal), and use these principles to explain the origin of negative refraction (but not necessarily a “negative index!”) in such systems. For simplicity, we begin by considering a 2D structure, following Ref. 87. In subsequent sections, we switch to a more realistic design that is still governed by similar principles.

A cross-section of an example 2D photonic crystal is illustrated in Fig. 5-1[left].
Figure 5-1: (Figure from Ref. 87.) [left] Schematic of reflection (blue) and refraction (red) of a plane wave incident (black) on a square lattice of dielectric rods (green) in air, for an interface with period $L = a\sqrt{2}$ in the diagonal (110) direction. Depending on the frequency, there may also be additional reflected and/or refracted waves due to Bragg diffraction. [right] Isofrequency contours in k-space at $\omega a/2\pi c = 0.276$ for air (black circle) and crystal (red contours), with the Brillouin zone in gray, for the example 2D photonic crystal shown at left. The group velocity $(VWk)$ directions at various $k$ points are shown as arrows (black/blue/red for incident/reflected/refracted waves). Because the wavevector component parallel to the interface is conserved, all reflected and refracted solutions (blue and red dots) must lie along the dashed fixed-$k_{||}$ line (running perpendicular to the interface).

The crystal, in this case, is a square lattice of dielectric ($\varepsilon = 11.4$) rods in air, with period $a$ and radius $0.2a$. The crystal is semi-infinite, terminated in the (11) (diagonal) direction as shown, so that the interface has period $L = a\sqrt{2}$ in the diagonal (11) direction. Light is incident from the side of the crystal. The physical principles are similar to those described by Luo et al., who achieved all-angle negative refraction (AANR) in 2D and 3D crystals (but using much larger refractive indices than are available to us) [116,118]. When an incident plane wave strikes an interface of a photonic crystal, some of the light will be reflected, some of the light can be transmitted or refracted, propagating at the angle of the group velocity within the
crystal. The way the incident radiation is refracted can be determined by analyzing the isofrequency diagram, a contour plot of \( \omega(k_x, k_y) \) at the incident \( \omega \), such as the one provided in Fig. 5-1(right).

By a corollary of Bloch’s theorem: in a linear system with discrete translational symmetry, the Bloch wavevector \( \mathbf{k} \) is conserved as light propagates, up to addition of reciprocal lattice vectors, in the relevant direction(s). Here, there is only translational symmetry along directions parallel to the interface, and so only the wave vector \( k_\parallel \) parallel to the interface is conserved. That is, suppose that the periodicity parallel to the interface is \( L \), and the incident plane wave has wavevector \( (k_\parallel, k_\perp) \) and frequency \( \omega \). Then, any reflected or refracted wave must also have frequency \( \omega \) and a wavevector \( (k_\parallel + 2\pi l/L, k_\perp') \) for any integer \( l \) and some \( k_\perp' \). Given the isofrequency diagram, it is straightforward to determine the states or directions in which the refracted waves will propagate. (The amplitudes of the refracted and reflected waves, on the other hand, depend on the surface termination and require a more detailed solution of the Maxwell equations.) The procedure is depicted in Fig. 5-1(right). For a chosen frequency, here \( \omega a/2\pi c = 0.276 \), we superimpose the (black) contour for the incident medium (air, a circle \( \omega = c|\mathbf{k}| \)) and the (red) contours for the transmitted medium (the photonic crystal).

The phase and group velocities of the incident wave are the same, since air is an isotropic and homogeneous medium. The wavevector \( \mathbf{k} \) points in the same direction as the group velocity (black arrow) on the incident contour, and makes an angle \( \theta \) with the surface normal. Then, to select modes with the same \( k_\parallel \), we draw a dashed line through the incident \( \mathbf{k} \) and perpendicular to the interface (here, along the \( \Gamma M \) direction). The place(s) where this dashed line intersects the photonic-crystal contours determines (determine) the refracted wave(s).

Although the fixed-\( k_\parallel \) line may intersect the photonic-crystal contours in several places, not all of these correspond to distinct refracted waves. We can eliminate any intersections (pink dots) corresponding to a group velocity (pink arrow) towards the interface from the crystal, as these violate our boundary conditions (the only incoming power is from the incident medium). In the example of Fig. 5-1(right),
The angles of incidence and refraction are labeled. \( k_M \) denotes the distance from the M point to the inscribed circle of the contour at the point where concavity around M transitions into convexity. We obtain the figure of merit \( C_M = \frac{k_M}{\omega} \).

At the interface between two ordinary homogeneous media, there can be at most one refracted wave — the graphical construction for us to conserve \( \omega \) and \( k_\parallel \) consists of two concentric circular contours centered around the \( \Gamma \) point. (The case with no refracted wave corresponds to total internal reflection as a wave travels from higher to lower index at an angle greater than the critical angle.) However, there are two ways one could get multiple refracted waves when light travels from a homogeneous medium to a photonic crystal. First, when the operating frequency is sufficiently high, our fixed-\( k_\parallel \) line could intersect multiple bands of the band structure. Second, our
fixed-$k_\parallel$ line could intersect a given contour at inequivalent points in different periodic unit cells. For example, if we had an interface at a different angle, the fixed $k_\parallel$, the line would not be at 45 degrees and could easily intersect the same contour at many different points. Conversely, there will be some cases for which there is no refracted wave. This happens also in homogeneous materials where Snell’s law is valid, in the case of total internal reflection, but here we have more opportunities for complete reflection due to the photonic band gaps—even if these are gaps over only a limited range of wavevectors. For example, in Fig. 5-1[right], we can see that for a larger incident angle $\theta$, our dashed line would not intersect the red photonic-crystal contour, leading to total reflection—even though this frequency lies outside the photonic band gap for other angles. For our negatively-refracting structure, we would like to have one refracted wave only, and we avoid the cases of multiple refracted waves and no refracted waves by design, as we will now illustrate.

### 5.2 Designing the structure

Our actual design is a photonic crystal slab: a 2D-periodic pattern with a finite thickness etched into some high-index layer on a lower-index substrate. Slab designs are experimentally attractive because they can be fabricated with conventional lithography. Fabrication constraints are especially important at visible wavelengths where the relevant lengthscales are small. We are further constrained by the available low-loss dielectric materials at visible wavelengths. (For example, silicon, which is used in most infrared photonics, is extremely lossy at visible wavelengths, since visible light has energies greater than the bandgap of silicon.) In particular, one of the highest available low-loss indices of refraction at visible wavelengths is found in silicon nitride ($\text{Si}_3\text{N}_4$), and so our design focused on a silicon nitride layer ($\varepsilon = 4.0678$ at 630 nm) sandwiched between two silicon dioxide ($\text{SiO}_2$, $\varepsilon = 2.12$) layers (on a silicon substrate, which adds a small downward leakage/absorption of light that is considered below). This is then etched with a 2D-periodic square array of air ($\varepsilon = 1$) holes (etched through both the silicon nitride and both oxide layers). The key question is then to
Figure 5-3: Band diagram around the irreducible Brillouin zone edge for our silicon nitride slab structure of height $h = 0.3a$ sandwiched between infinite silicon dioxide above and below and a square lattice of holes with radius $r = 0.25a$ drilled in. The grey shaded region is the light cone, the extended modes propagating in air. The discrete modes below are guided bands localized in the nitride slab. We operate at a frequency of $0.4127 \cdot 2\pi c/a$, corresponding to a visible wavelength of 630 nm. The calculation was performed using MPB [89].

determine the optimal achievable parameters (period, hole radius, and thicknesses) for our application.

Similar devices designed for infrared frequencies are often SOI structures with a layer of silicon ($\varepsilon \approx 12$) on silicon dioxide ($\varepsilon = 2.25$). There, the index contrast is so high that the guided mode lies mainly in the high-index silicon layer and will see very little of the substrate layer underneath [87]. For visible wavelengths in our case, however, the nitride/oxide index contrast is relatively low, so that the guided mode (in the $z$ direction, see below) penetrates into the oxide layers a lot more than it does for SOI. Therefore, we sandwich the high-index nitride layer with oxide layers above and below to create a more symmetric structure. This allows us to obtain a clear distinction between even and odd eigenmodes (with respect to the $z = 0$ midplane) so
that we can use one polarization without mixing. (An even mode is “TE-like,” with \(E\) mostly in-plane and \(H\) mostly out-of-plane, while an odd mode is the “TM-like” reverse [87].) (Another possibility would be a suspended membrane structure, which is possible for silicon at infrared scales [87], but is much more challenging at visible lengthscales.)

Since we have a photonic crystal slab instead of a true 2D structure with infinite height, light is confined in the nitride layer by index guiding in the third \((z)\) direction, and we must exclude modes that lie above the light cone because they radiate away. Thus, a desired design of a photonic crystal slab that exhibits negative refracting behavior has convex contours around the M point, which is where the light cone leaves maximal space, as opposed to, for example, the \(\Gamma\) point. Note that even for a cutoff-free guided mode (which does not exist here because of the substrate, which violates the conditions of Chapter 4), the guided mode ceases to exist at the \(\Gamma\) point because at zero frequency, we no longer have wave solutions. As shown in Fig. 5-3, only the first guided mode is present for structures that we consider at the operating frequency, so it is sufficient to consider only the isofrequency diagram for this band, plotted in the first Brillouin zone \((|k_x|, |k_y| \leq \pi/a)\). (This is by design—coupling to modes in other bands would lead to multiple refracted rays.) We would like to maximize the convex region around the M point for negative refraction. We first recall from Fig. 5-2 that we come in from air, which has \(\omega(k_x, k_y)/c = |k|\) (its isofrequency curve is a circle with radius \(\omega/c\)). We come in at the angle \(\theta_i\) to the normal and determine the direction of refraction by conserving \(\omega\) and \(k_\parallel\) (up to \(2\pi \ell/L\), \(L = a\sqrt{2}\) is the periodicity parallel to the interface)—that is, we can only couple to modes along the dashed line in Fig. 5-2. (If the air contour were large enough, the dashed line would intersect additional crystal contours, beginning with the contours at the other two M points in the first Brillouin zone. This would correspond to multiple refracted rays, or different \(\ell\) orders. We avoid this situation by design.)

There are two key criteria that are sufficient to guarantee single-beam AANR [118].

1. The constant-frequency contour of the photonic crystal (here, the contour around M) at the operating frequency is convex, with an inward-pointing group veloc-
ity (a consequence of the contour being around a frequency \textit{maximum}, i.e. the negative curvature of $\omega(k)$, i.e. “negative photonic effective mass” [118]).

2. All incoming wavevectors from air at such a frequency are included within the constant-frequency contour of the photonic crystal, so that there can be a single refraction due to the crystal. i.e. the frequency is small enough. That is, in our case the contour around M at the operating frequency (in units of $2\pi c/a$) has a radius in k-space equal to that in air around $\Gamma$.

In addition, if one wished to have only a single \textit{reflected} beam in air (and a single transmitted beam in air through a finite crystal back into air), then the frequency must be below the diffraction limit: we must have $\frac{\omega L}{2\pi c} = \frac{L}{\lambda} \leq 0.5$ [87, 118].

Although Ref. 118 was able to satisfy all of these conditions in two dimensions with high dielectric contrast ($\varepsilon = 12$), the second criterion turns out to be infeasible at the low 4:1 $\varepsilon$ contrast available in our application. Decreasing the contrast has two effects. First, it decreases the gap at the Brillouin zone edge, which shrinks the contour around the M point (it shrinks the region of strong negative curvature). Second, decreasing the indices pushes the photonic-crystal bands up in frequency at a fixed $a$, or equivalently forces one to increase $a$ and hence shrink the Brillouin zone (diameter $2\pi/a$) at a fixed operating frequency - this shrinks the entire isofrequency diagram of the photonic crystal and hence shrinks the relevant M contour. Thus, working with lower indices of refraction makes the M contour smaller, in two ways, relative to the air contour. At silicon nitride indices, this seems to make AANR infeasible. Instead, we try to obtain negative refraction over as wide a range of incident angles as possible.

In particular, the key question determining the range of incident angles that can be negatively refracted is the size of the largest convex contour around M relative to the operating frequency. The size of this contour can be quantified by the radius $k_M$ around the M point of the inscribed circle for the largest convex contour, as shown in Fig. 5-2. The figure of merit is then $C_M = k_M/\omega$. If contours from other frequencies are also shown (suppressed for clarity here), one would observe a transition from
concavity to convexity, and the contour is flat at this transition point, where an unusual effect known as supercollimation can be achieved (as we describe in more detail below).

Optimization for negative refraction, i.e. maximizing $C_M$, was first performed by simulating a structure with infinitely high oxide layers above and below the high index nitride layer with holes in all the layers. This is valid as long as the oxide layers actually fabricated are thick enough, because all guided modes in this structure decay into the oxide and then the air above and the silicon substrate below it. If the oxide layers are thick enough, the field patterns and thus frequencies would not be impacted significantly. More discussion will follow as to how we determine the required thickness of the oxide layers. The parameters are the period size, $a$, radius-to-period ratio, $r$, and the thickness-to-period ratio of the nitride layer, $h$. We optimize for these ratios instead of actual dimensions (i.e., we set $a$ to 1 for now), since Maxwells equations are scalable, such that we can scale the actual dimensions for the desired operation frequency (as discussed below) [87].

(The silicon substrate below has a negligible impact on the dispersion relation of the modes in the nitride layer, so it was omitted from these calculations for simplicity. The silicon substrate was included in the transmission simulations below, where it affects the propagation loss.)

We note some trends of the contours here (all in terms of relative $r$ and $h$):

1. The frequencies $\omega$ increase as we increase $r$ for fixed $h$, and decrease as we increase $h$ for fixed $r$. This is expected from the variational principle [87] that as the structure has a higher "effective" dielectric index, frequencies decrease.

2. For a given value of $h$, $C_M$ increases and reaches some optimum before decreasing again as we increase $r$ from 0 (no holes) to 0.5 (holes touching each other). This is accompanied by the observation that the contours look "more round" around M as we increase $r$, but frequencies increase uniformly as we increase $r$, thus we can see where the tradeoff comes from.

3. As we move toward M from $\Gamma$, the contours look more convex, but the contours
are smaller in k-space (since they are closer to M). Thus, as we increase the frequency of operation for a given design, we obtain negative refraction over a smaller range of angles, but the magnitude of the (negative) angles of refraction increases for a given incident angle. This is a tradeoff between the range of angles we can observe negative refraction and the extent of the negative refraction.

4. Since the contours are not perfectly circular, some of them are convex in certain directions in k-space but concave in others; therefore, some angles of incidence give positive refraction, while others give negative refraction. This reflects the nature that there is no effective “index” with which we can describe the negatively refracting behavior. In Fig. 5-6, there is positive refraction for small incident angles but negative refraction for larger incident angles.

Based on these trends, the optimized parameters are $h/a = 1.05$ and $r/a = 0.35$ at a dimensionless frequency $f$ of 0.370 (in units of $2\pi c/a$). For an operating wavelength of $630\text{nm}$, we obtain the physical period of our design $a = f\lambda = 0.370 \times 630\text{nm} = 233 \text{ nm}$. Note that light will couple to whatever modes of the system that have conserved $\omega$ and $k_\parallel$ values, and which have the same direction of energy transport. Therefore, we need to prevent coupling into other modes. As we increase $h$, there will be higher modes of similar transverse characteristics with more nodes in $z$, whose frequencies further decrease as we increase $h$. Thus we cannot choose an arbitrarily large thickness of the nitride. A finite-difference time domain (FDTD) simulation (performed using MEEP [139]) indicates that a point source close to the slab incident from the side emerges as a collimating beam, demonstrating supercollimation Fig. 5-5.

Supercollimation is the propagation of optical beams without spatial spreading [87, 98, 152]. In a homogeneous medium, light beams spread out, or “diffract”, as they propagate, and the amount of spreading is proportional to the wavelength divided by the beam size [167]. This occurs because a localized light source consists of Fourier components in many different directions. These components travel in different directions, leading to beam diffraction. This is analogous to the position-momentum
uncertainly relation in quantum mechanics [166]. In Fig. 5-2, one observes that the convex band around the M point is quite flat. At the point of transition from concavity to convexity, the band is perfectly flat. At such an operating frequency, a diffracting beam becomes collimated and propagates without spreading. Using photonic crystals, beams only a few wavelengths wide have been observed to travel for almost one centimeter with no spreading for infrared wavelengths [152]. We shall return to the subject of supercollimation at the end of the chapter.

Due to fabrication constraints, the above ideal structure could not be fabricated. There are a number of other considerations we need to take into account:

1. Fabrication constraints do not allow radius-to-period ratios of greater than 0.25. Since performance increases monotonically with this ratio, peaks at 0.35 and decreases with further increase of this ratio, we adopt 0.25 as our ratio, and a comparison of the performances will be shown below.

2. Fabrication constraints dictate a maximum 300 nm total of etched height in the top oxide layer, nitride layer, and the bottom oxide layer. We initially designed our structure by simulating with a symmetric (infinite) structure having the same oxide thickness on top of and below the nitride layer—hence all the guided modes in that system would be either even or odd. In a real system, we lose this perfect symmetry since we have a silicon substrate below and air on top. With our even mode light source, we utilize the structure’s first even mode. The loss of perfect symmetry would lead to coupling of unwanted odd modes and degrade the performance. To avoid coupling into odd modes and into the silicon substrate, we would like to preserve the symmetry as much as possible by maximizing the thicknesses of the top and bottom oxide layers. Given our operating wavelength of 630 nm, and with these new constraints, we redesigned the structure to have $h/a = 0.3$ and to operate at the dimensionless frequency of 0.4127, which translates to a physical period of $a = 0.4127 \times 630 \text{ nm} = 260 \text{ nm}$. The physical nitride height is 78 nm, leaving us with top and bottom oxide heights of 111 nm each. The isofrequency diagram of this design is show in
Fig. 5-6. Negative refraction is observed.

3. We analyzed the even/odd characteristics of the first “odd-like” band (i.e., the first band whose electric field is mostly odd with respect to z), assuming infinite bottom oxide thickness, with the top layer of oxide having thickness in increments of 0.1 units of a. We found that when this latter thickness, $h_{\text{top}}/a > 0.4$ (around 100nm for our design), then the first “odd-like” mode couples less than 1% to our incident light (chosen to be even in z) and causes minimal loss. If $h_{\text{top}} > 0.2$ (50nm), then the first “odd-like” mode will cause less than 4% of loss.

4. Numbers of rows and columns of holes should be maximized as long as the loss due to material absorption is not significant, so that the periodicity becomes close to “infinite”. Nitride has an extinction coefficient $\alpha$ of $0.0524 \mu m^{-1}$, which corresponds to a decay of 0.1 of the original power in $44 \mu m$. Therefore, as long as we keep the dimension in the perpendicular direction to the edges facing the input/output beams to $< 0.1$ of that, we should not experience significant loss due to material absorption.

5. Surface terminations can affect the transmission of power by refraction through the structure. We can terminate the 2D periodicity at the center of the hole, in the middle between two lines of holes, or anywhere in between. Time domain simulations must be used to get this information, since frequency domain simulations only give us what the modes of the system are.

Based on these constraints, as well as the trends and observations we described, we designed the test structures to operate at different distances from the M point. We can make many different combinations of period sizes and radii for our wafer of fixed height. Therefore, we choose a combination of operating points that give good behavior around the flat contour region with a relatively large range of incident angles that give small extents of negative refraction, and operating points that exhibit larger extents of negative refraction in a smaller range of angles (closer
to the M point). After determining the height of the nitride layer by the incident wavelength 630nm, we go to smaller $h/a$ ratios (increasing the physical period $a$) in order to go toward the M point in the contour plot (where the curves are more "round") gradually. The testing of these can give us an idea of a good compromise.

Practically, we have a fixed wafer height for all the layers. Increasing the period decreases the normalized height of the nitride layer, thus increasing the normalized frequency, moving us closer to the M point. Since $a = f\lambda$, increasing both $a$ and $f$ (as a result of increasing $a$) does not change the physical operating wavelength by much. Recall that we tend to get a smaller range of angles that exhibit NIB but larger magnitudes of these refracted angles, we are thus exploring different operating points in k-space in slightly different structures. Due to fabrication imperfections, this is a very good way to test for NIBs.

We checked for the desired NIB using FDTD simulations using MEEP [139]:

1. Incoming plane waves at an angle: We send in plane waves at various angles and compare the angles of refraction with findings from frequency simulations. Some results are shown in Fig. 5-7.

2. Point source for observing focusing/supercollimation: Using FDTD simulations, we can observe the field patterns of what happens on the other side of the slab when we put a point source on one side of the slab. Some results are shown in Fig. 5-8 and Fig. 5-9.

For each set of the parameters, our collaborators fabricated the structures described above, with the number of holes in the $y$ direction between about 2 and 20 to reduce intensity loss, and the number of holes in the $x$ direction being 5 to 8 times as the number of holes in the $y$ direction so as to ensure that the periodicity appears "infinite" as seen by the incoming light.
The negatively-refracting and focusing photonic crystal slab structures that we designed have been fabricated and are shown in Fig. 5-10. Listed below are the simulated angles of refraction for a range of parameters that cover the range of design parameters fabricated (with the desired operating frequencies):

First, let us consider a wavelength that is slightly too large (too small a frequency) to couple to a purely convex contour, so that incident waves at some small angles are positively refracted. In particular, Table 5.1 shows the results for a structure with \( a = 260 \text{ nm} \) and \( h = 76 \text{ nm} \), operating at 634nm (normalized frequency 0.41).

<table>
<thead>
<tr>
<th>Incident</th>
<th>2.0</th>
<th>4.0</th>
<th>6.0</th>
<th>8.0</th>
<th>10.0</th>
<th>11.0</th>
<th>12.0</th>
<th>13.0</th>
<th>14.0</th>
<th>15.0</th>
<th>16.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Refracted</td>
<td>+0.7</td>
<td>+1.4</td>
<td>+1.9</td>
<td>+1.8</td>
<td>+0.6</td>
<td>-0.9</td>
<td>-2.9</td>
<td>-6.7</td>
<td>-13.5</td>
<td>-26.5</td>
<td>-51.3</td>
</tr>
</tbody>
</table>

Table 5.1: Angles of refraction for oxide-nitride-oxide PC slab with \( a = 260 \text{ nm} \), \( h = 76 \text{ nm} \), operating wavelength=634nm (normalized frequency 0.41)

The same structure operating at 630 nm (normalized frequency 0.4127), which also couples to a slightly non-convex contour, gives negative refraction from about 10 to 14.4 degrees. Results are shown in Table 5.2.

<table>
<thead>
<tr>
<th>Incident</th>
<th>2.0</th>
<th>4.0</th>
<th>6.0</th>
<th>8.0</th>
<th>10.0</th>
<th>11.0</th>
<th>12.0</th>
<th>13.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Refracted</td>
<td>+0.7</td>
<td>+1.3</td>
<td>+1.6</td>
<td>+1.2</td>
<td>-0.5</td>
<td>-2.5</td>
<td>-5.8</td>
<td>-12.0</td>
</tr>
</tbody>
</table>

Table 5.2: Angles of refraction for oxide-nitride-oxide PC slab with \( a = 260 \text{ nm} \), \( h = 76 \text{ nm} \), operating wavelength=630 nm (normalized frequency 0.4127)

By the time the wavelength goes down to 600 nm (normalized frequency 0.4337), the M contour has become purely convex, and so all incident angles are negatively refracted, if they are refracted at all, but angles beyond about 10 degrees are reflected. Results are shown in Table 5.3.

<table>
<thead>
<tr>
<th>Incident</th>
<th>2.0</th>
<th>4.0</th>
<th>6.0</th>
<th>7.0</th>
<th>8.0</th>
<th>10.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Refracted</td>
<td>-0.2</td>
<td>-1.2</td>
<td>-6.4</td>
<td>-10.5</td>
<td>-22.0</td>
<td>-89.3</td>
</tr>
</tbody>
</table>

Table 5.3: Angles of refraction for oxide-nitride-oxide PC slab with \( a = 260 \text{ nm} \), \( h = 76 \text{ nm} \), operating wavelength=600 nm (normalized frequency 0.4337)

Results are shown in Table 5.4 for the same structure operating at 591 nm (normalized frequency 0.44).
Table 5.4: Angles of refraction for oxide-nitride-oxide PC slab with $a=260$ nm, $h=76$ nm, operating wavelength=591 nm (normalized frequency 0.440)

Results for $a=275$ nm and $h=76$ nm operating at 634 nm (normalized frequency 0.4337) are shown in Table 5.5.

Table 5.5: Angles of refraction for oxide-nitride-oxide PC slab with $a=275$ nm, $h=76$ nm, operating wavelength=634 nm (normalized frequency 0.4337)

Results for $a=275$ nm and $h=71$ nm operating at 634 nm (normalized frequency 0.4337) are shown in Table 5.6.

Table 5.6: Angles of refraction for oxide-nitride-oxide PC slab with $a=275$ nm, $h=71$ nm, operating wavelength=634 nm (normalized frequency 0.4337)

Finally, results for $a=280$ nm and $h=71$ nm operating at 634 nm (normalized frequency 0.4416) are shown in Table 5.7.

The reason why we have listed different operating frequencies is that it is the normalized frequency (period/wavelength)—not the actual frequency—that determines the properties, and we note that during fabrication there may be slight non-uniformities that would change the effective normalized frequency.

## 5.3 Experimental Results

Our collaborators at Agiltron Inc. fabricated the structures described above with various air-hole diameters and periods, shown in Fig. 5-10 [209]. This way, NIBs could be evaluated under different conditions even if the fabricated structures differ from our design due to fabrication tolerance.
Table 5.7: Angles of refraction for oxide-nitride-oxide PC slab with \(a=280\) nm, \(h=71\) nm, operating wavelength=634 nm (normalized frequency 0.4416)

<table>
<thead>
<tr>
<th>Incident</th>
<th>3.0</th>
<th>4.0</th>
<th>5.0</th>
<th>6.0</th>
<th>7.0</th>
<th>8.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Refracted</td>
<td>-0.5</td>
<td>-1.2</td>
<td>-2.9</td>
<td>-6.0</td>
<td>-12.8</td>
<td>-28.8</td>
</tr>
</tbody>
</table>

NIB has been observed in our samples at the visible wavelength of 634 nm. Figure 5-11 shows some measured results from four different chips. A lensed fiber was placed horizontally on the left side of the PC structure. In Fig. 5-11[a], the PC occupies the entire probe region. The incident angle \(\theta_i = -6.30^\circ\), and the theoretical refraction angle is \(-3.04^\circ\). However, the observed refraction angle is \(\theta_r = -0.52^\circ\). In Fig. 5-11[b]–[d], the PC has a smaller period and the probe light enters the SiO\(_2\)/Si\(_3\)N\(_4\)/SiO\(_2\) waveguide portion (no air holes) first and then enters photonic crystal portion.

Note that \(k_{||}\) is conserved as we enter from air into the waveguide region, as well as from the waveguide region into the PC. Even though there is an intermediate region through which the light travels, our negative refraction predictions, applied to the incident angle in air and the refracted angle in the crystal, are not affected. Our calculations show that the unpatterned waveguide at 634 nm has an effective index \((|k|c/\omega)\) of 1.577, so we can use this value in Snell’s law to convert the incident angle \(\theta_w\) measured in the waveguide into an incident angle \(\theta_i = \sin^{-1}(1.577 \sin \theta_w)\) in the air.

There is negative refraction in all cases shown in Fig. 5-11 except possibly for Fig. 5-11[a] where the refracted angle was too small to determine its sign with confidence. To our knowledge, these results represent the lowest-loss NIB at visible wavelengths compared to existing research. Our extinction coefficient is 0.0524 \(\mu m^{-1}\), which is almost an order of magnitude better than the state-of-the-art value of 0.43 \(\mu m^{-1}\) reported in Ref. 206.

The precise angles of refraction at given wavelengths, however, inevitably differ slightly from theoretical predictions, simply because the structures differ slightly from theoretical design. (For example, the holes in Fig. 5-10 are clearly not etched completely vertically, equivalent to a hole radius that is a few percent off from the the-
oretical design.) As given in the tables of theoretical refraction angles, the refracted angle depends quite sensitively on the wavelength, and any shift in the frequencies of the bands due to fabrication errors will cause a correspondingly large shift in the refraction angle. (In fact, this large sensitivity is related to something called a “super-prism” effect that occurs in very flat bands [97].)

One interesting possibility that has yet to be fully explored experimentally, is to use this design to achieve visible-wavelength supercollimation rather than negative refraction, where the best supercollimation is achieved for normal incidence. Supercollimation relies on having a flat PC contour that is as large as possible, in order to collimate as many Fourier components of a given beam as possible—this is essentially equivalent to maximizing the largest convex contour around M, so our design is also an optimized supercollimator. Previous experimental work on supercollimation has focused instead on infrared wavelengths [152]. In the case of our design in Fig. 5-6 (period $a = 260$ nm), the first completely flat band appears to occur between normalized frequencies of 0.414 and 0.42, corresponding to incident wavelengths between 628 nm and 619 nm.
Figure 5-4: A zoomed-in isofrequency plot for a silicon nitride photonic crystal slab of thickness $h = 1.05a$ and radius of air holes $r = 0.35a$ sandwiched between silicon dioxide of infinite height above and below. ($a$ is the period of the square lattice.) Directions of group velocity are displayed, giving refracted ray directions (on the 0.370 contour, closed to the 0.371 contour, which is labeled).
Figure 5-5: A finite-difference time domain (FDTD) simulation confirms supercollimation behavior in our structure. Nitride thickness =245 nm, period=233 nm and radius= 78nm. A monochromatic point source with even parity, operating at the flat region of the first even band, is used. We observe a nice collimated beam on the other side. This is a cross section of the center of the nitride slab along the z direction. The x-dimension of the diagram shown is about 10 μm, so the collimated beam has a transverse extent of about 1 μm.
Figure 5-6: A zoomed-in isofrequency plot for a oxide-nitride-oxide sandwich structure with \( h = 0.3a \) and \( r = 0.25a \). The red lines indicate the incoming wave direction. Angles of incidence shown here at 0, 4, 8, and 12 degrees. The refracted ray directions are given by the black arrows (on the 0.4127 contour, close to the 0.4197 contour, which is labeled). Physical height of the nitride layer is 78nm, the period is 260nm, and the hole radius is 65nm.
[a] Incident angle of 4 degrees. From approximate ray-tracing, the angle of refraction is close to $-1^\circ$.

[b] Incident angle of 7 degrees. The predicted angle of refraction is close to $0^\circ$.

Figure 5-7: Gaussian beams approximating plane waves with incident angles of 4 and 7 degrees come in from the side of the structure with a nitride height of 78 nm, period of 260 nm, hole radius of 65 nm (top view).
Figure 5-8: This structure has a nitride height of 78 nm, period of 260 nm, with 200 nm of oxide on top and 200 nm of oxide below the nitride. The bottom layer sits on a silicon substrate. We show below the top view of the field pattern of the output field, i.e., just above the structure, assuming incident comes from the bottom of the figure. The $y = 0$ position is the point just emerged from the photonic crystal slab. We observe interesting spot patterns that appear periodically in the $y$ direction. This is possibly due to the asymmetry in the actual structure, since we did not observe this when we used an infinite oxide layers above and below in our simulation. We can observe multiple intensity maxima (images) along $y$. The image at 0.6 $\mu$m from the slab is not degraded by much from the one at 0.25 $\mu$m, close to the slab, and even the third image at 1 $\mu$m is still quite distinguishable. The image distance of the third image is around the same as the object distance (around 1 $\mu$m).
Figure 5-9: This is the same structure as in Fig. 5-8 except that the heights of the top and bottom oxide layers are now decreased from 200 nm to 111 nm. Here, the stray spots on the side of the first main image along x=0 seem to overtake the image. The image at 0.65 μm is still distinguishable, albeit more weakly. However, the image at 1 μm has disappeared into the background noise. The degradation of performance can be explained as follows: Electric fields tend to concentrate in higher dielectric regions. Now that the bottom oxide thickness has been reduced, and recall that with our thin nitride thickness (set by various fabrication constraints), the photonic modes in this structure have fields that are not well localized in the nitride layer, or even the oxide layers, since the constraints are such that the total etch thickness can only be up to 300 nm. Thus, we get a lot of fields extending outside of the oxide-nitride-oxide sandwich, and the field profile will be skewed toward the silicon substrate instead of toward the air, lowering the frequency of the guided modes from the case with thicker oxide layers on top and below. We are therefore operating at a frequency above the flat band, since the flat band frequency of the structure has shifted down.
Figure 5-10: Fabricated structures.
Figure 5-11: NIB observed on different 2D photonic crystal slabs at a wavelength of 634nm.
Chapter 6

Conclusions

In this thesis, I have investigated the interaction of light and matter in three main contexts: potential brain injury caused by mechanical blast waves, guidance conditions in microstructured waveguides and their implications on the design of single-polarization single-mode waveguides, and the design of low-loss negatively-refracting dielectric structures for visible wavelengths using photonic crystal slabs. These are all very exciting topics; and, looking forward, there are still interesting questions to be explored.

In the brain project, the most important work would be more accurate measurements of the piezoelectric properties of human skull in realistic conditions (appropriate humidity and temperatures in “fresh” samples). It would be interesting to determine any spatial variation of the piezoelectric coefficient $d$ across the thickness of the bone or in different regions of the skull; for example, any rapid variation in the magnitude or orientation of the piezoelectric tensor $d$ across sutures between cranial bones would lead to greatly increased $\rho$ at these joints. If the magnitudes are similar, but the orientation switches rapidly, any charges created may cancel each other out and not be effective as a source of electric field. More accurate information on the piezoelectric tensor is crucial to the quality of any computational models built. Second, a biofidelic model with more divisions of zones in head might be helpful. For example, skin and fat are currently in one zone, but they have very different properties, and the uncertainty of electrostatic calculations will vary greatly depending on how the
zoning is done. Finally, since dielectric properties are frequency-dependent, it would also be desirable to have a more fully time-resolved simulation that takes into account material dispersion more carefully.

For the “proof” project, a number of interesting directions to pursue are discussed in Sec. 4.1.5, Sec. 4.2.8, and Sec. 4.3.5. A big-picture direction to pursue would be to prove localization conditions in bandgaps for the electromagnetic case. We have observed that going from the simple 2D ground state proof to the electromagnetic case (especially for general periodic claddings) introduced the need for many algebraic manipulations as well as careful limiting procedures; going from the ground state proof to the gap-localization proof in quantum mechanics also complicated the mathematics greatly. Proving 2D localization for gap-guidance in Maxwell’s equations is therefore a challenge not for the faint of heart.

Finally, our design of the NIB material for visible wavelengths appears to be quite successful. Hopefully there will be more researchers to take advantage of the materials we have chosen to continue this promising work and use the basic photonic crystal slab to build more complex devices, pushing negative refraction and supercollimation down to visible wavelengths, so as to benefit imaging and lithography applications, to name just a few.
Bibliography


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