Understanding Photonic Band Gaps via Symmetry and Perturbation Theory

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We study band gaps in photonic crystals, which are fundamental to understanding numerous phenomena such as light confinement and omnidirectional mirrors. To begin, we introduce the reader to the Hermitian eigenproblem underpinning electromagnetism, showing how many of the ideas of standard quantum mechanics carry over to this domain. In particular, we adapt the tools of symmetry and perturbation theory to the electromagnetic context. Finally, we use these tools to explain photonic band gaps.

I. INTRODUCTION

Some of the most interesting optical devices are photonic crystals, which have periodic structure in their dielectric permittivity. This periodicity leads to a number of important physical phenomena, such as omnidirectional reflection and light confinement. To understand these phenomena, it is crucial to understand the band structure of photonic crystals, and in particular the formation of photonic band gaps.

In this paper, we approach this phenomenon using the tools of symmetry and perturbation theory. First, we show that in a source-free setting, the solution modes to Maxwell’s equations can be found by solving a Hermitian eigenproblem, in close analogy with the time-independent Schrodinger equation of quantum mechanics (Section II A). This allows us to bring many of the techniques of quantum mechanics to bear on this domain.

In particular, we study translational symmetry, in both the cases of discrete (Section III A) and continuous (Section III B) translational symmetry. Our key motivating question involves both these cases: what happens when we start with a system that has continuous translational symmetry (i.e. a homogeneous medium) and “turn on” a periodic perturbation that immediately imposes discrete translational symmetry instead?

Our claim is that a band gap is a natural result of this transition. To explain this, we adapt first-order perturbation theory to electromagnetism (Section II B). We then apply it to a periodic perturbation of a multilayer film, thereby providing an intuitive, physical explanation for the origin of band gaps (Section IV).

We emphasize that we work at a length scale significantly larger than the Bohr radius, such that classical electromagnetism applies. Throughout this paper, our focus will be on adapting the ideas from quantum mechanics to this new context, thereby showing how their wide applicability to arbitrary Hermitian eigenproblems.

II. EIGENPROBLEMS IN ELECTROMAGNETISM

We work in a source-free setting, where there are no free charges or currents. Further, we assume that the magnetic permeability is always $\mu_0$. We begin by writing down Maxwell’s equations in this setting.

\[
\nabla \cdot \mathbf{E} = 0 \quad (1)
\]

\[
\nabla \cdot \mathbf{B} = 0 \quad (2)
\]

\[
\nabla \times \mathbf{E} = -\frac{dB}{dt} \quad (3)
\]

\[
\nabla \times \mathbf{B} = \varepsilon(r) \frac{d\mathbf{E}}{dt} \quad (4)
\]

Note that Maxwell’s equations are linear in the electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$. Furthermore, note that they are time-independent. Thus, assuming that $\varepsilon(r)$ is also time-independent, by time-invariance symmetry we can restrict our attention to the case of frequency “modes” where $\mathbf{E}$ and $\mathbf{B}$ can be decomposed into a spatial component and a time-varying exponential,

\[
\mathbf{E}(r, t) = \mathbf{E}(r)e^{-i\omega t}, \quad (5)
\]

\[
\mathbf{B}(r, t) = \mathbf{B}(r)e^{-i\omega t}. \quad (6)
\]

We are now ready to state our concrete problem: given the spatial distribution $\varepsilon(r)$ of the dielectric permittivity, what are the possible frequency modes $\mathbf{E}(r), \mathbf{B}(r)$? This is analogous to the problem in time-independent quantum mechanics, where we are given a potential $V(r)$ and asked to find the stationary states $\psi(r)$.

As in quantum mechanics, we can derive an eigenproblem, where the Hermitian operator depends on the given quantity, which is $\varepsilon(r)$ in this case. First, note that by
Eq. (5) and Eq. (6)
\[
\frac{dE}{dt} = -i\omega E, \quad (7) \\
\frac{dB}{dt} = -i\omega B. \quad (8)
\]
Here, we suppress the dependency on \(r\) in writing the modes \(E\) and \(B\), just as one often thinks of \(\psi\) in quantum mechanics more abstractly as an element of a Hilbert space. Now, the Maxwell equations Eq. (3) and Eq. (4) become
\[
\nabla \times E = -\frac{dB}{dt} = i\omega B \\
\nabla \times B = -i\omega \varepsilon(r)E. \quad (9)
\]
\[
\nabla \times \frac{1}{\varepsilon(r)} \nabla \times B = \omega^2 B. \quad (11)
\]
Instead using Eq. (9) to eliminate \(E\) in Eq. (10), we obtain
\[
\nabla \times \nabla \times E = \omega^2 \varepsilon E. \quad (12)
\]
Although one might expect Eq. (11) and Eq. (12) to be essentially the same, they are actually quite different. In particular, Eq. (11) is a familiar eigenproblem in \(B\): the right-hand side is a scalar multiplied by \(B\). In contrast, in Eq. (12), there are non-trivial linear operators on both sides of the equation.

In the remainder of this section, we will see why both of these equations are useful to keep in mind. In particular, we will see that Eq. (11) is a Hermitian eigenproblem; this allows us to borrow many concepts from quantum mechanics, such as the existence of a complete set of solution modes, without re-derivation. On the other hand, Eq. (11) is difficult to work with perturbatively; we will use Eq. (12) to derive a quantitative expression for first-order perturbation theory.

A. Hermitian Eigenproblem

To make the eigenproblem more explicit, we denote the linear operator of Eq. (11) on the left-hand side as \(\hat{\Theta}\), so that
\[
\hat{\Theta}B = \omega^2 B. \quad (13)
\]
Before formally declaring Eq. (13) an eigenproblem, we need to take a step back and define the Hilbert space on which \(\Theta\) acts. Note that we have not yet used Eq. (2), which gives us another constraint on \(B\). Thus, we form a Hilbert space consisting of all vector fields \(F\) defined over our volume of interest (which is either all of space or a finite region with periodic boundary conditions) that also obey a transversality condition,
\[
\nabla \cdot F = 0. \quad (14)
\]
As in the standard treatment of quantum mechanics, we neglect functional analysis issues.

Our inner product over the Hilbert space assumes a similar form to that of quantum mechanics. However, since we are dealing with vector fields, we cannot perform a scalar multiplication at each spatial coordinate. Instead, we take the natural generalization, which is the dot product of the vectors at each spatial coordinate,
\[
\langle F \cdot G \rangle = \int F^\ast(r) \cdot G(r)dV. \quad (15)
\]
Equipped with this inner product, we can show that \(\hat{\Theta}\) is Hermitian,
\[
\langle \hat{\Theta}F, G \rangle = \langle F, \hat{\Theta}G \rangle \quad (16)
\]
The proof is by integration by parts, which we omit from this treatment as it does not offer much intuition. The Hermicity of \(\hat{\Theta}\) has deep physical implications, notably the idea of Lorentz reciprocity, which states that one can interchange the positions of current sources and electric field measurements in any setup, and keep the relationship between the two the same.

B. Electromagnetic Perturbation theory

In this section, we develop first-order, non-degenerate perturbation theory for electromagnetism.

Eq. (12) is actually a generalized eigenproblem, with Hermitian operators on both sides. (For readers who have seen the wave equation in electromagnetism before, this is the same equation in disguise.) While it was easier to work directly with the traditional eigenproblem to apply the theory from quantum mechanics directly, when working perturbatively it is easier to deal with Eq. (12), as we do not have to deal with the differentiation of the \(1/\varepsilon(r)\) term inside the curl operator.

We are interested in the effect of a perturbation \(\Delta \varepsilon(r)\) to the initial dielectric permittivity \(\varepsilon_0(r)\). Expanding everything as a power series in a small parameter \(\lambda\),
\[
\varepsilon(r) = \varepsilon_0(r) + \lambda \Delta \varepsilon(r) \quad (17) \\
E(r) = E_0(r) + \lambda \Delta E(r) + O(\lambda^2) \quad (18) \\
\omega = \omega_0 + \lambda \Delta \omega + O(\lambda^2), \quad (19)
\]
where \(E_0\) and \(\omega_0\) represent an unperturbed frequency mode and angular frequency, respectively. We drop the superscripts in the usual treatment since we are only expanding to first order. Substituting into Eq. (12) and
implicitly dropping terms of order $O(\lambda^2)$,
\begin{equation}
\nabla \times \nabla (E_0 + \lambda \Delta E) \approx (\omega_0 + \lambda \Delta \omega)^2 (\varepsilon_0 + \lambda \Delta \varepsilon) (E_0 + \lambda \Delta E).
\end{equation}

Matching the terms of order $\lambda$,
\begin{equation}
\nabla \times \nabla \times E = 2\omega_0 \Delta \varepsilon E_0 + \omega_0^2 \Delta \varepsilon E_0 + \omega_0 \varepsilon_0 \Delta E.
\end{equation}

As in the standard treatment, we make the useful choice of normalization
\begin{equation}
\langle E, \Delta E_0 \rangle = 0.
\end{equation}

Then, taking the component of $E_0$ on both sides of Eq. (22),
\begin{equation}
\langle E_0, \nabla \times \nabla \times E \rangle = 2\omega_0 \Delta \varepsilon \langle E_0, \varepsilon E_0 \rangle + \omega_0^2 \langle E_0, \Delta \varepsilon E_0 \rangle.
\end{equation}

By the Hermicity of the double curl operator $\nabla \times \nabla \times$, the left hand side evaluates to 0, and so we derive
\begin{equation}
\Delta \omega = \frac{-\omega_0 \langle E_0, \Delta \varepsilon E_0 \rangle}{\omega_0^2 \langle E_0, \varepsilon E_0 \rangle}.
\end{equation}

As a basic sanity check on Eq. (25), we note that $\omega$ decreases when $\Delta \varepsilon$ is everywhere positive. This makes sense, because the speed of light $v$ in a medium is proportional to $1/\sqrt{\varepsilon}$ and thus decreases, so from the plane-wave relation $\omega = \nu \cdot d$, we would expect $\omega$ to also decrease.

But Eq. (25) also affords us new insight. In particular, it tells us that modes which are concentrated in regions where $\Delta \varepsilon$ is the largest / most positive will decrease the most in frequency, while modes which are concentrated in regions where $\Delta \varepsilon$ is the smallest / most negative will increase the most in frequency.

\section{III. Symmetries}

Now that we have a Hermitian eigenproblem, we can apply what we know from quantum mechanics to understand the effect of symmetries in the electromagnetic case, which play a crucial role in understanding photonic band gaps.

\subsection{A. Discrete translational symmetry}

We first discuss discrete translational symmetry. Discrete translation symmetry is important because photonic crystals have periodic structures, meaning that the dielectric permittivity $\varepsilon(r)$ is invariant under translation by integer multiples of a vector $d$. Expressed algebraically, this symmetry implies that
\begin{equation}
[\hat{\Theta}, T_d] = 0,
\end{equation}
where $T_d$ is the operator that translates by $d$, i.e. $T_d(B(r)) = B(r - d)$. Thus, we know that $T_d$ and $\hat{\Theta}$ can be simultaneously diagonalized, and in particular each frequency mode $B(r)$ must be a member of an eigenspace of $T_d$.

What are these eigenspaces? We must have that $B(r + d) = CB(r)$ for some constant $C$, which is close to but not quite periodicity. To strip away this multiplicative constant, we extract an exponential prefactor $e^{ik_\|r_\|d}$ from $B(r)$. Here, $r_d$ is the component of the position vector in direction $d$ and $k_d$ is a scalar. We can then write,
\begin{equation}
B(r) = e^{ik_\|r_\|d} B_{k_d}(r),
\end{equation}
where $B_{k_d}(r)$ is truly periodic, satisfying $B_{k_d}(r) = B_{k_d}(r + d)$. This is the famous Bloch’s theorem of quantum mechanics, which as we see applies in general to any Hermitian eigenproblem with discrete translational symmetry.

Notice that $k_d$ identifies the eigenspace, but there is some freedom in its choice. For example, if we choose $k_d = \frac{2\pi}{d}$, then the exponential $e^{ik \cdot r}$ would itself be invariant under shifts in $d$, i.e. $e^{ik \cdot r}$, and thus could be folded into $B_{k_d}(r)$. To avoid this issue, we can restrict the possible choices of $k_d$ to the range $-\pi/|d| < k_d \leq \pi/|d|$, which defines the so-called “Brillouin zone”.

When there are multiple vectors which exhibit discrete translational symmetry, which we shall call lattice vectors, we can add a prefactor for each of them. Or more simply, we can combine all of them into a single wave vector $k$ that belongs to the span of the lattice vectors (which explains our previous notation $k_d$), such that
\begin{equation}
B(r) = e^{ik \cdot r} B_k(r),
\end{equation}
where $B_k(r)$ is periodic for all lattice vectors. Once again, we can define a Brillouin zone that contains a complete set of wave vectors $k$ that lead to a unique eigenspace.
where $B_k(r)$ only depends on the component of $r$ orthogonal to all directions of continuous translational symmetry.

### 1. Snell’s Law

To understand the power of exploiting symmetry, let us provide a direct proof of Snell’s law using continuous translational symmetry. Suppose that a light wave is incident at an interface, as shown in Fig. 2, with wavevector in the $xz$-plane. Eq. (29) immediately tells us that the $x$-component $k_x$ of the wave vector is conserved for both the reflected and refracted rays. Since the magnitude of the wave vector is proportional to the refractive index (from classical wave optics), we have

$$n_1 \sin \theta_1 = \frac{n_1 k_x}{n_1 \omega/c} = \frac{c k_x}{\omega} = \frac{n_2 k_x}{n_2 \omega/c} = n_2 \sin \theta_2.$$

So Snell’s law is an immediate consequence of continuous translational symmetry of the system in the direction along the interface.

### C. Connection between continuous and discrete symmetry

For both continuous and discrete symmetry, a wave vector $k$ is used to identify the eigenspace. However, there are two crucial differences.

1. The function $B_k(r)$ is much more tightly constrained in the continuous case, as it must have no dependence whatsoever on the directions with translational symmetry. In contrast, $B_k(r)$ only needs to be periodic with respect to the lattice vectors in the discrete case.

2. Each choice of wave vector $k$ gives a unique eigenspace in the continuous case, but not in the discrete case, where instead the wave vectors that generate all unique eigenspaces form a Brillouin zone.

### IV. APPEARANCE OF PHOTONIC BAND GAPS

We now give an intuitive, physical explanation of the origin of photonic band gaps using the tools we have developed so far. Imagine starting with a homogeneous medium and “turning on” a periodic perturbation $\Delta \varepsilon$ such that we get a structure with discrete periodicity. The motivating question is: how does the continuous spectrum suddenly obey the rules of discrete periodicity, and how do band gaps appear? We will aim to give a satisfactory answer to this question by working perturbatively.

The precise setup is shown in Fig. 3. The photonic crystal consists of alternating slabs of permittivities $\varepsilon$ and $\varepsilon + \Delta \varepsilon$, where each slab has width $d/2$. We consider the case of on-axis propagation, where waves propagate along the $x$-axis. The electric field, along which we orient the $y$-axis, then depends only on $x$.

Before perturbation, the solutions for a particular $k = k_x$ are two-fold degenerate, given as

$$E(x) = (Ae^{ikx} + Be^{-ikx}) \hat{y}.$$

For simplicity, let us focus on symmetry in a single direction $d$. From the second point above, we can understand that a particular wave vector in the Brillouin zone with magnitude $k_d$ in the discrete case is formed by “folding together” the wave vectors in the continuous case with magnitudes

$$k_d + \frac{2\pi n}{|d|}$$

for integer $n$. Intuitively, this folding of an infinite set of states in one permits greater freedom in the function $B_k(r)$, explaining point 1.

This discussion will prove useful when we discuss the appearance of band gaps in Section IV.
Photonic band gap

Breaking of degeneracy

| k = −π/d | k = 0 | k = π/d |

FIG. 4: Formation of band gap

Initially, all possible values of $\omega = kc/\varepsilon$ are allowed, so there is no band gap.

Before applying perturbation theory, we need to decide which of these degenerate subspaces we are interested in studying to reveal the band gap behaviour. This requires some physical insight. Recall from Eq. (32) of Section III C that we can think of the wave vectors as “folding over” when transitioning to the discrete case. Also recall from Section III A that, once discrete translational symmetry is imposed, each Bloch wave vector $k = \mathbf{k}_z$ will correspond to a countable (i.e. discretely spaced) set of solution modes.

The diamond shape in Fig. 4 shows the implications of these two ideas, where the first two Bloch solutions are depicted for each $k$. As the perturbation is turned on, the sides of this diamond will evolve continuously. From the picture, we can see that the only place a band gap can be formed is at the energy corresponding to the edge of the Brillouin zone, where $k = \pm \pi/d$ (neglecting higher order band gaps that come from considering the third Bloch states, and so on). So, let us apply perturbation theory to the eigenspace given by Eq. (33) for the choice $k = \pi/d$.

Although this is strictly speaking a case of degenerate perturbation theory, we are only interested in the first-order change. So Eq. (25) is still applicable, as long as we apply it to the “good basis” for the eigenspace in which $\Delta \varepsilon$ is diagonal. (Here, we slightly abuse notation by using $\Delta \varepsilon$ to refer both to the scalar change in $\varepsilon$ for each layer, and as the function $\Delta \varepsilon(x)$ that gives the perturbation of $\varepsilon(x)$ over all of space.)

Given that the good basis has size two, by the variational theorem we can find its elements by considering the solution modes which maximize and minimize the quadratic form $\langle \mathbf{B}, \Delta \varepsilon \mathbf{B} \rangle$. For $\Delta \varepsilon > 0$, this quadratic form is maximized by a mode that peaks in the layer with permittivity $\varepsilon + \Delta \varepsilon$, and it is minimized by a mode that peaks in the layer with permittivity $\varepsilon$. For $\Delta \varepsilon < 0$, it is the opposite way around, but the modes are still the same. We depict these two modes in Fig. 5: this is our good basis. Setting $x = 0$ at the left end of a layer with permittivity $\varepsilon + \Delta \varepsilon$, the electric fields of the modes are given by

$$E_1(x) = \sin^2 \left(\frac{\pi x}{d} + \frac{\pi}{4}\right)$$

$$E_2(x) = \sin^2 \left(\frac{\pi x}{d} - \frac{\pi}{4}\right).$$

We apply non-degenerate perturbation theory (Eq. (25)) to $E_2(x)$, considering only the range $0 \leq x < d$ due to the periodic structure.

$$\frac{\Delta \omega_2}{\omega} = -\frac{1}{2} \int_0^d |E_2(x)|^2 \Delta \varepsilon(x) dx$$

$$= -\frac{1}{2} \frac{\Delta \varepsilon}{\varepsilon} \int_0^{1/2} \sin^2 \left(\pi x + \frac{\pi}{4}\right) dx$$

$$= -\frac{1}{2} \frac{\Delta \varepsilon}{\varepsilon} \int_0^{1/2} \left(1 - \cos \left(2\pi x + \frac{\pi}{2}\right)\right) dx$$

$$= -\left(\frac{1}{4} + \frac{1}{4\pi} \left[\sin \left(2\pi x + \frac{\pi}{2}\right)\right]_0^{1/2}\right) \frac{\Delta \varepsilon}{\varepsilon}$$

By an identical argument, we have

$$\frac{\Delta \omega_1}{\omega} = -\left(\frac{1}{4} - \frac{1}{2\pi}\right) \frac{\Delta \varepsilon}{\varepsilon}.$$ 

Immediately, we see that $\Delta \omega_2 \neq \Delta \omega_1$: the degeneracy has been broken, as shown in Fig. 4, forming a band gap. Note that this agrees with the intuition presented at the end of Section II B: the electric fields of the two modes are concentrated in regions with different permittivities, so we would expect the degeneracy to be broken.

We can obtain a quantitative expression for the size of the photonic band gap by subtracting the two,

$$\frac{\Delta \omega}{\omega} = \frac{\Delta \omega_1 - \Delta \omega_2}{\omega} \frac{1 \Delta \varepsilon}{\varepsilon},$$

obtaining a quantitative expression for the relative height of the gap, to the first-order approximation.

V. CONCLUSION

We have shown how to adapt the formalism of quantum mechanics to the electromagnetic context. This shows the generality of the ideas of quantum mechanics, and also highlights new problems that can arise in different contexts, such as generalized eigenproblems and vector-valued fields satisfying transversality constraints.

By drawing an analogy to quantum mechanics, we have introduced the reader to the field of photonic crystals. Using electromagnetic perturbation theory, we have explained how a photonic band gap is formed. Although it
is true that explicit non-perturbative forms can be given for the band gap, the value of our perturbative treatment is the physical intuition it provides into why a gap arises, and how it is fundamentally linked to the transition from continuous to discrete translational symmetry.

This work could be extended by considering two- and three-dimensional photonic crystals, and the interesting physical phenomena that can arise in these settings, such as a complete photonic band gap in all settings.