On the Role of Symmetries in the Theory of Photonic Crystals

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We discuss the role of the symmetry induced by complex conjugation $C$ in the theory of photonic crystals. Borrowing the jargon of the classification theory of topological insulators, we show that $C$ is a “particle-hole-type symmetry” rather than a “time-reversal symmetry” if one consider the Maxwell operator in the first-order formalism where the dynamical Maxwell equations can be rewritten as a Schrödinger equation. We justify by an analysis of the band structure why the first-order formalism seems to be more appropriate than the second-order formalism. Moreover, based on the Schrödinger formalism, we introduce a class of effective (tight-binding) models called Maxwell-Harper operators. Some considerations about the breaking of the “particle-hole-type symmetry” in the case of gyrotropic crystals are added at the end of this paper.

Key words: photonic crystal, gyrotropic effect, Harper-Maxwell operator, complex electromagnetic fields

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1 Introduction

Roughly speaking, a photonic crystal (PhC) is to light what a crystalline solid is to an electron. Based on this analogy, experiments have been proposed which realize “quantum-like systems” in PhCs. On the other hand, many well-known effects from solid state physics have been anticipated in PhCs. That is how edge currents in PhCs have been predicted \cite{rh08,oo09,ljs12} and observed \cite{wcj08,wcj09,flg11,prs12,rpz13}.

However, this correspondence between electrodynamics and quantum mechanics is not one-to-one, and there are aspects where these differences become crucial. A priori there is no way of knowing when it breaks down or even if “analogous” phenomena have the same explanation. For instance, the analogy to the Bloch electron suggests that the existence of topologically protected edge states in PhCs can be explained by the bulk-edge correspondence \cite{hat93,kso4} (proved under various levels of generality in \cite{hat93,kso4}). Its validity is still an open problem, and it cannot merely be assumed but eventually needs to be established by a first-principles derivation.

This paper focuses on the role of symmetries, because breaking inversion and “time-reversal symmetry” becomes crucial for the observation of topological effects. The main purpose of this work is to explain why we have put time-reversal symmetry in quotation marks, and our main points are:

(1) The dynamical Maxwell equations can be recast in the form of the “Schrödinger equation” \eqref{schrodinger}, a first-order equation in time. While it is true that complex conjugation

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C is a “time-reversal symmetry” of the second-order formulation of the Maxwell equations (3.1), in the parlance of classification theory of topological insulators \([AZ97; SRF+08]\) it is a particle-hole symmetry (PH symmetry) of the first-order equation. This symmetry is present if and only if the electric permittivity \(\epsilon\) and the magnetic permeability \(\mu\) are tensors with real entries.

(2) Since the Schrödinger equation is a first-order equation in time, it is the first-order classification of \(C\) as PH symmetry which matters for the subsequent analysis. The Maxwell operator (cf. equation (2.4)) is of symmetry class \(D\) rather than \(AI\), so even in non-gyrotropic media, Chern numbers (or other topological obstructions) associated to single, isolated bands need not be zero!

(3) Nevertheless, the presence of the PH symmetry explains the absence of topological effects in non-gyrotropic media: electromagnetic fields are real observables, and real fields emerge as linear combinations of conjugate pairs of Bloch functions. Thanks to the PH symmetry, the total Chern number associated with a pair of conjugate states is zero because the Chern numbers of symmetrically related bands are equal in magnitude but have opposite sign. That means for symmetrically chosen families of bands one is back again in the setting of symmetry class \(AI\) where one of the authors has recently proven the absence of all topological obstructions \([DG14]\).

(4) Thus, the study of effective dynamics in photonic crystals (see e.g. \([OMN06; RH08; DL14a]\)) is a bona fide multiband problem since single bands can never support real states. That is particularly significant for approaches which have derived effective ray optics equations, because effective single band equations do not describe the evolution of physical states.

(5) We propose the Maxwell-Harper operator (5.1) for a conjugate pair of bands as a simple model operator for non-gyrotropic PhCs in analogy to the usual Harper operator. It is a \(2 \times 2\) matrix operator and exists even if the bands carry non-zero Chern charge.

In what follows, we will derive and expound on these assertions.

The paper is roughly structured as follows: we will first reformulate the Maxwell equations as a Schrödinger-type equation in Section 2, derive the frequency band spectrum and expound on the significance of complex conjugation. Then we will juxtapose first- and second-order formalism in Section 3. After that we will show how complex conjugation as a PH symmetry induces a relation between the Chern numbers of symmetrically related bands (Section 4). The Maxwell-Harper operator is introduced in Section 5. We close the paper by a discussion of gyrotropic materials where the electric permittivity \(\epsilon\) and the magnetic permeability \(\mu\) are hermitian matrix-valued functions with non-zero imaginary parts.
2 The first-order Schrödinger formalism

The claim that light and a quantum particle behave similarly is fundamentally a statement about their dynamics. The propagation of electromagnetic waves in a linear, three-dimensional medium are governed by the two dynamical Maxwell equations,

\[
\begin{align*}
\epsilon \partial_t E(t, x) &= \nabla \times H(t, x), \\
\mu \partial_t H(t, x) &= -\nabla \times E(t, x),
\end{align*}
\]

whereas the absence of sources is described by

\[
\begin{align*}
\nabla \cdot \epsilon E(t, x) &= 0, \\
\nabla \cdot \mu H(t, x) &= 0.
\end{align*}
\]

The properties of the material enter through the electric permittivity tensor \(\epsilon\) and the magnetic permeability tensor \(\mu\). While most materials are non-gyrotropic, i.e. \(\epsilon(x)\) and \(\mu(x)\) are real-symmetric, there are cases when \(\epsilon(x)\) and \(\mu(x)\) are hermitian with non-zero imaginary part (see e.g. [YCL99; WLF+10; KRL+10; EG13]). Throughout this paper, we assume that \(\epsilon\) and \(\mu\) are positive, bounded with bounded inverse. To simplify the notation we shall refer to \(w = (\epsilon, \mu)\) as material weights and use \(\bar{w} = (\bar{\epsilon}, \bar{\mu})\) to denote the complex conjugate weights.

To the best of our knowledge, the idea to express the dynamical Maxwell equations as a Schrödinger equation

\[
i \partial_t \Psi = M \Psi
\]

originated in a paper by Birman and Solomyak [BS87]. Here, the electromagnetic field \(\Psi = (E, H)\) plays the role of the wave function and the Maxwell operator

\[
M_w = \begin{pmatrix}
0 & +i \epsilon^{-1} \nabla^\times \\
-i \mu^{-1} \nabla^\times & 0
\end{pmatrix}
\]

takes the place of the quantum Schrödinger operator \(H = \frac{-i\hbar}{2m}(\nabla^2 + V)\). Throughout the paper we use the short-hand \(\nabla^\times E = \nabla \times E\), e.g. \(\nabla^\times E = \nabla \times E\) denotes the curl. The material weights \(w = (\epsilon, \mu)\) also enter into the definition of the scalar product

\[
\langle \Psi, \Psi' \rangle_w = \langle E, E' \rangle + \langle H, H' \rangle = \int_{\mathbb{R}^3} \text{d}x \left( E(x) \cdot \epsilon(x) E'(x) + H(x) \cdot \mu(x) H'(x) \right),
\]

and the corresponding Hilbert space \(L^2_w(\mathbb{R}^3, \mathbb{C}^6)\) is \(L^2(\mathbb{R}^3, \mathbb{C}^6)\) equipped with the weighted scalar product \(\langle \cdot, \cdot \rangle_w\). Note that complex conjugation is contained in \(\nabla \cdot w := \sum_{j=1}^3 \nabla_j w_j\).
This weighted scalar product provides a decomposition of electromagnetic waves into longitudinal and transversal component: a quick computation shows that gradient fields are \( \langle \cdot, \cdot \rangle_w\)-orthogonal to fields satisfying (2.1) \cite[Section 3]{DL14b}. Moreover, the Maxwell operator is hermitian, \( \langle \Psi, M_w \Psi' \rangle_w = \langle M_w \Psi, \Psi' \rangle_w \), and consequently, the time-evolution \( e^{-itM_w} \) is unitary. This leads to the conservation of field energy \[
E(E,H) = \frac{1}{2} \int_{\mathbb{R}^3} dx \left( E(x) \cdot \varepsilon(x) E(x) + H(x) \cdot \mu(x) H(x) \right) = \frac{1}{2} \| (E,H) \|_w^2. \] (2.6)

### 2.1 The frequency band picture

The particularity of photonic crystals is that the material weights \( (\varepsilon, \mu) \) are periodic with respect to some lattice \( \Gamma = \text{span}_\mathbb{Z} \{ e_1, e_2, e_3 \} \) spanned by three (non-unique) fundamental vectors. Now one proceeds as if \( M_w \) were a periodic Schrödinger operator: we employ the Bloch-Floquet-Zak transform \( (Z \Psi)(k, y) = \sum_{\gamma \in \Gamma} e^{-ik(y+\gamma)} \Psi(y+\gamma) \) to change representation \( (Z \) maps onto the space-periodic part of Bloch functions). As explained in \cite[Section 3]{DL14b} the operator \( M_w \) is unitarily equivalent to a family of Maxwell operators

\[
M_w(k) = \begin{pmatrix} 0 & -\varepsilon^{-1}(-i\nabla+k)^\varepsilon \\ +\mu^{-1}(-i\nabla+k)^\mu & 0 \end{pmatrix} \] (2.8)

depending on crystal momentum \( k \) where \( M_w(k) \) acts on \( \Gamma \)-periodic electromagnetic fields \( \psi = (\psi^E, \psi^H) \). This gives rise to Bloch functions \( \varphi_n(k) \) and Bloch frequency bands \( \omega_n(k) \),

\[
M_w(k) \varphi_n(k) = \omega_n(k) \varphi_n(k). \] (2.9)

\( M_w(k) \) has a flat band \( \omega(k) = 0 \) due to unphysical gradient fields; Bloch functions associated to non-zero frequency bands are automatically source-free \cite[Section 3]{DL14b},

\[
(\nabla + ik) \cdot \varepsilon \varphi_n^E = 0, \quad (\nabla + ik) \cdot \mu \varphi_n^H = 0.
\]

Schematically, the frequency band spectrum looks as in Figure 2.1: there are 2 “ground state bands” with approximately linear dispersion at \( k \approx 0 \). Apart from \( k = 0 \), bands do not touch \( \omega = 0 \). Note that there are bands of positive and negative frequency; the signs correspond to outgoing and incoming complex Bloch waves. This can already be inferred from (2.4), the Maxwell operator looks very similar to a massless Dirac operator. Note that the figure depicts the band spectrum of a non-gyrotropic PhCs, leading to the point symmetry in the spectrum; with the exception of this symmetry the band spectra of gyrotropic PhCs share all other features.
2 The first-order Schrödinger formalism

\[ A + n^2 n^4 n^3 n^2 n^1 n^3 n^4 A - B - B + p p k \]

Figure 2.1: A sketch of a typical band spectrum of \( M_w(k) \) for a non-gyrotropic photonic crystal (i.e. \( \varepsilon \) and \( \mu \) are real). The 2+2 ground state bands (±\( n_1 \)) with linear dispersion around \( k = 0 \) are blue. Positive frequency bands are drawn using solid lines while the lines for the symmetrically-related negative frequency bands are in the same color, but dashed.

2.2 Complex conjugation as a particle-hole symmetry

Complex conjugation \( C \Psi(x) := \overline{\Psi(x)} \) induces a relation between \( M_w \) and the Maxwell operator \( M_{w^c} \) with complex conjugate material weights,

\[ C M_w C = -M_{w^c}. \quad (2.10) \]

Consequently, Maxwell operators \( M_w \) for non-gyrotropic media (\( \overline{w} = w \)) are of class \( D \) in the Altland-Zirnbauer classification scheme \([AZ97; SRF+08]\), meaning \( C \) acts as a particle hole symmetry. \( C \) cannot be interpreted as implementing time-reversal,\(^1\)

\[ C e^{-it M_w} C = e^{it CM_{w^c}} C = e^{-it M_{w^c}}. \quad (2.11) \]

Instead, complex conjugation interchanges incoming and outgoing complex waves; This was first noted in \([Ber82, Section III]\) for purely homogeneous media where the material weights are constant, but was not linked explicitly to complex conjugation.

\(^1\)Note that \( C \) is not an anti-unitary map between \( L_2^2(\mathbb{R}^3, C^6) \) and itself but only as a map \( L_2^2(\mathbb{R}^3, C^6) \) and the Hilbert space with conjugate weights \( L_2^2(\mathbb{R}^3, C^6) \).
2.3 Physical states in non-gyrotropic photonic crystals

Translating equation (2.10) to the Bloch-Floquet-Zak representation involves the PH symmetry $C^Z = ZCZ^{-1}$,

\[ (C^Z \varphi)(k, y) = \overline{\varphi(-k, y)}, \]  

(2.12)

and leads to

\[ CM_w(k)C = -M_w(-k). \]  

(2.13)

In other words, we have $M_w(k)\varphi_n(k) = \omega_n(k)\varphi_n(k)$ if and only if $M_w(k)(C^Z \varphi_n)(k) = -\omega_n(-k)(C^Z \varphi_n)(k)$.

Equation (2.13) explains the point symmetry in the band spectrum of non-gyrotropic materials where $w = w$: *frequency bands come in pairs* $(\omega_n(k), -\omega_n(-k))$ with Bloch functions $(\varphi_n(k), (C^Z \varphi_n)(k))$ (dashed and solid lines of the same color in Figure 2.1). These Bloch waves are necessarily complex, because $\varphi_n$ and $C^Z \varphi_n$ are eigenfunctions to frequency bands of different sign.

2.3 Physical states in non-gyrotropic photonic crystals

Electromagnetic waves $(E, H)$ are real and transversal, i.e. they satisfy $C(E, H) = (E, H)$ and the source-free equations (2.2). By definition Zak transforms of such functions are “real” with respect to $C^Z = ZCZ^{-1}$, i.e.

\[ C(E, H) = (E, H) \iff C^Z Z(E, H) = Z(E, H). \]

The action of $C^Z$ given by (2.12) is no longer just pointwise complex conjugation, and to avoid confusion we call functions $\psi(k)$ in Bloch-Floquet-Zak representation Real if $(C^Z \psi)(k) = \overline{\psi(-k)} = \psi(k)$. This is also consistent with the terminology used in the theory of Real vector bundles [Ati66, DG14].

Let us focus on states that are localized in a narrow frequency range, i.e. states associated to a family of Bloch bands which do not cross or merge with other bands. In the simplest case, we only need to consider a single, non-degenerate bands $\omega^+ > 0$ and its symmetric twin $\omega^-(k) = -\omega^+(-k)$ whose Bloch functions $\varphi_-(k) = (C^Z \varphi_+)(k) = \varphi_+(-k)$ are related by complex conjugation. Then the two Real solutions

\[
\begin{align*}
\psi_{Re}(k) &= \frac{1}{\sqrt{2}} (\varphi_+(k) + \varphi_-(k)) \\
\psi_{Im}(k) &= \frac{1}{i\sqrt{2}} (\varphi_+(k) - \varphi_-(k))
\end{align*}
\]

\footnote{Even for ground state bands, i.e. the bands with linear dispersion around $k = 0$, a real Bloch basis can only be chosen at $k = 0$.}
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are Real and Imaginary part of $\varphi_+$; if we introduce the Real part operator \( \text{Re} Z = \frac{1}{2}(1 + C^2) \) and the Imaginary part operator \( \text{Im} Z = \frac{1}{2i}(1 - C^2) \), then we can succinctly write $\psi_{\text{Re}} = \sqrt{2} \text{Re} Z \varphi_+$ and $\psi_{\text{Im}} = \sqrt{2} \text{Im} Z \varphi_+$. Physical states associated to the band $\omega_+$ are real linear combinations of $\psi_{\text{Re}}$ and $\psi_{\text{Im}}$, and these real linear combinations always depend on both, $\varphi_+$ and $\varphi_-$. Hence, finding effective dynamics for physical states is a multi-band problem. In that sense, previous works which concerned the derivation of effective single-band dynamics in analogy to solid state physics [OMN06; RH08; EG13] give an incomplete picture.

2.4 Two- vs. three-dimensional PhCs

All of our arguments generalize to two-dimensional PhCs as the 2d Maxwell operator is a restriction of (2.4). Thus, also in two dimensions $C$ is a particle-hole symmetry and frequency bands on the two-dimensional Brillouin zone come in conjugate pairs.

To make our arguments self-contained, let us sketch a derivation (see also [Kuc01, Chapter 7.2.5] for the isotropic case): suppose the material weights $w = (\epsilon, \mu)$ are of both of the form

\[
w = \begin{pmatrix} w_1 & u + iv & 0 \\ u + iv & w_2 & 0 \\ 0 & 0 & w_3 \end{pmatrix} = \begin{pmatrix} \psi & 0 \\ 0 & w_3 \end{pmatrix}
\]

i.e. they factor into two blocks. As a consequence the fields in the $x_1 x_2$-plane and along the $x_3$-direction are orthogonal, e.g.

\[\langle (E_1, E_2, 0), (\epsilon(0, 0, E_3)) = 0,\]

and similarly for the magnetic field. Moreover, electric fields of the form $(E_1, E_2, 0)$ drive the dynamics for the magnetic field only along the $x_3$-direction, \( \partial_t \mathbf{H} = -\mu^{-1} \nabla \times \mathbf{E} = (0, 0, \partial_3 \mathbf{H}_3) \). Hence, if we start with a transverse electric (TE) mode \( ((E_1, E_2, 0), (0, 0, H_3)) \), the time-evolved state will be of the same form. One can repeat the same arguments for transverse magnetic (TM) modes \( ((0, 0, E_3), (H_1, H_2, 0)) \).

Now let us impose a second assumption on the material weights, namely that they are independent of $x_3$. Then we can make a product ansatz $\Psi(x_1, x_2, x_3) = \Phi(x_1, x_2) e^{ik_3 x_3}$ for the electromagnetic fields where the component depending on $x_3$ is just a plane wave. The 2d Maxwell operator emerges after choosing $k_3 = 0$ (meaning the fields are independent of $x_3$), i.e.

\[M_{w,2d} = \begin{pmatrix} 0 & +i\epsilon^{-1} (\partial_1, \partial_2, 0)^x \\ -i\mu^{-1} (\partial_1, \partial_2, 0)^x & 0 \end{pmatrix}\]
where \((\partial_1, \partial_2, 0)^* \mathbf{E} = (\partial_1, \partial_2, 0) \times \mathbf{E}\). Electromagnetic fields of finite energy are now elements of \(L^2_\omega(\mathbb{R}^2, \mathbb{C}^6)\) with a weighted scalar product defined analogously to (2.5).

The block structure of the material weights leads to a block decomposition of the Maxwell operator \(M_{\omega, 2d} = M_{\text{TE}} \oplus M_{\text{TM}}\) induced by splitting electromagnetic fields into TE and TM modes,

\[
L^2_\omega(\mathbb{R}^2, \mathbb{C}^6) = L^2_{\text{TE}} \oplus L^2_{\text{TM}}.
\]

These two operators can be compactly written as \(3 \times 3\)-matrix-valued operators, e. g.

\[
M_{\text{TE}} = \begin{pmatrix}
0 & 0 & +i\varepsilon^{-1}(
\begin{pmatrix}
+\partial_2 \\
-\partial_1
\end{pmatrix}


0 & 0 & -i\mu_3^{-1}\partial_2 \\
+i\mu_2^{-1}\partial_2 & -i\mu_3^{-1}\partial_1 & 0
\end{pmatrix}
\end{pmatrix}
\]

is the form of the Maxwell operator for TE modes \((E_1, E_2, H_3)\). This block structure also means that TE and TM components are independent, e. g. one can compute their (two-dimensional) frequency bands and Bloch functions separately. Given that we have derived the 2d Maxwell operator from the full, three-dimensional Maxwell equations, \(M_{\omega, 2d}\) inherits properties such as the particle hole-type symmetry. Consequently, also 2d frequency bands and Bloch functions come as conjugate pairs. And while the particle hole-type symmetry does not force single bands to be topologically trivial (the Chern number associated to \(\varphi_n\) need not be zero), real and imaginary part of \(\varphi_n\) are. From the viewpoint of topological insulators this is not surprising: the 2d Maxwell operator is of class D in the Altland-Zirnbauer classification scheme, so one expects to find a \(\mathbb{Z}\)-valued topological index.

### 3 First- vs. second-order formalism

Most of the time, at least implicitly, the second-order equation

\[
(\partial_t^2 + M_{\omega}^2) \Psi = 0
\]

is considered instead of (2.3). From a practical point of view, this has a number of advantages, most importantly, electric and magnetic components decouple and one obtains two second-order PDEs. And only one of the two equations need to be solved. Moreover, in two dimensions this leads to two scalar equations, one for the TM and another for the TE modes. These simplifications allow for a more efficient treatment.

The eigenvalue problem that is usually solved in other works reads

\[
M_{\omega}(k)^2 \varphi_n(k) = (\lambda_n(k))^2 \varphi_n(k)
\]
where $\lambda_n = |\omega_n(k)|$ is taken to be positive. This eigenvalue problem is subtly different, because the information whether the Bloch wave is outgoing ($\omega_n > 0$) or incoming ($\omega_n < 0$) is discarded.

If we take the absolute value of the spectrum of our fictitious Maxwell operator from Figure 2.1, the much more convoluted frequency band picture of Figure 3.1 emerges. Compared to the signed band spectrum, many artificial band crossings appear (the points $X_j$ and $Y_j$). If one were to label frequency bands by magnitude in Figure 3.1, then the relabeled Bloch functions are discontinuous at these artificial points of intersection. Some of these artificial crossings suggest that bands are coupled even though they are not (e.g. bands $n_{\pm 2}$ intersects with bands $n_{\pm 4}$ in Figure 3.1). In fact, there would be no isolated bands: due to $\omega_n(k) \leftrightarrow -\omega_n(-k)$ every eigenvalue in the spectrum of Figure 3.1 has even degeneracy at $k = 0$. Even if the spectral information can somehow be reconstructed, labeling bands in this fashion artificially alters the topology of the Bloch bands. Given that topological terms also enter into the dynamical equations, e.g. the Berry curvature appears in the ray optics equations, labeling bands properly is crucial.

Also in the second-order formalism, the information contained in the sign of $\omega_n$ is critical when one wants to reconstruct solutions to the dynamical problem. The similarity
of (3.1) to the wave equation suggests to rewrite it as

\[(\partial_t + iM_w(k)) (\partial_t - iM_w(k)) \Psi = 0\]

in Bloch-Floquet-Zak representation, and we see that any solution is a linear combination of an outgoing and an incoming wave.

4 Role of complex conjugation as a symmetry

Clearly, for non-gyrotropic materials where \(M_w = M_{\text{re}}\), complex conjugation leaves (3.1) invariant. To call \(C\) a “time-reversal symmetry” is misleading, though: in view of equation (2.11) time-reversal

\[(E(t), H(t)) \mapsto (E(-t), -H(-t))\]

is not implemented by \(C\) as in the case of quantum mechanics. Instead, the presence of \(C\) as a symmetry states that initially real electromagnetic fields stay real under time evolution. In gyrotropic PhCs this is no longer true, initially real fields acquire a non-zero imaginary part over time.

Moreover, if one wants to transfer arguments and techniques from quantum mechanics, it is the classification of the first-order operator that matters, and complex conjugation acts as a PH symmetry there. This difference becomes crucial when one wants to study topological properties of Bloch bands, e.g. Chern numbers.

Symmetries can ensure the topological triviality of a family of bands: assume we are given a projection \(\pi(k)\) for which

\[C \pi(k) C \pi(-k)\]

holds, then it is well-known that the associated first Chern class vanishes.

To show that the PH symmetry does not necessarily imply (4.1), it is instructive to review the argument which establishes (4.1) in the Schrödinger case where \(CH(k)C = H(-k)\). Suppose we are given a contiguous family of energy bands \(\sigma_{\text{rel}}(k) = \bigcup_{n \in I} \{E_n(k)\}\) indexed by \(I = \{n_{\text{min}}, \ldots, n_{\text{max}}\}\) that is separated from all others by a gap, e.g. the yellow \((\pm n_2)\) or the violet bands \((\pm n_3)\) in Figure 2.1. Then the projection onto the associated eigenspaces

\[\pi(k) = \sum_{n \in I} |\varphi_n(k)\rangle \langle \varphi_n(k)| = \frac{i}{2\pi} \int_{\gamma(k)} dz \left( H(k) - z \right)^{-1} \]

\[\quad \quad \quad = \frac{i}{2\pi} \int_{\gamma(k)} dz (D(k) - z)^{-1} \]

11
can either be expressed as a sum of rank-1 projections or as a Cauchy integral where the contour $\gamma(k)$ encloses only $\sigma_{\text{rel}}(k)$. Conjugating the projection with $C$ yields

$$C \pi(k) C = -\frac{i}{2\pi} \int_{\gamma(k)} dz \left(C H(k) C - z\right)^{-1}$$

because $C H(k) C = H(-k)$ implies $\sigma_{\text{rel}}(-k) = \sigma_{\text{rel}}(k)$ is enclosed by $\gamma(k)$. Hence, the first Chern numbers associated to $\sigma_{\text{rel}}(k)$ vanish.

For non-gyrotropic photonic crystals, this is false: Let us pick a contiguous, separated family of positive frequency bands $\sigma_+(k) = \bigcup_{n \in I} \omega_n(k)$, and define the collection of symmetrically related bands $\sigma_-(k) = \bigcup_{n \in I} -\omega_n(-k)$ as well as the associated projections $\pi_{\pm}(k)$. Then instead of (4.1) a modification of the arguments in equation (4.2) yields

$$C \pi_+(k) C = \pi_-(k),$$

from which we deduce that the Chern numbers of $\pi_{\pm}$ are equal in magnitude, but are of opposite sign [DL14a, Remark 4]. However, there are a few projections which do have trivial Chern numbers, for instance, (4.1) holds for $\pi(k) = \pi_+(k) + \pi_-(k)$. Also the projections $|\psi_{\text{Re}}(k)\rangle\langle\psi_{\text{Re}}(k)|$ and $|\psi_{\text{Im}}(k)\rangle\langle\psi_{\text{Im}}(k)|$ onto $\text{Re}^{Z} \varphi_n$ and $\text{Im}^{Z} \varphi_n$ satisfy (4.1) by construction, and thus, Chern numbers associated to real states vanish. This explains the absence of topological effects in non-gyrotropic PhCs.

Hence, the strategies proposed to observe topological effects (see e.g. [RH08; OO09]) are in principle correct but need to be modified: physical states are real which forces one to include conjugate pairs of bands. As argued in [DL14a, Section 5], the simplest model for a PhC with broken inversion and PH symmetry would include two symmetrically related bands rather than a conical intersection. The phenomena in graphene-like PhCs are due to two complementary mechanisms, namely the lack of conjugate pairs of Bloch functions and the opening of the conical intersection at the $K$- and $K'$-points which can change the topological charge carried by each band (see [OO09; DL13]).

5 The Maxwell-Harper approximation for non-gyrotropic PhCs

Usually, the frequency bands and Bloch functions are only obtainable numerically for given choices of $\epsilon$ and $\mu$, and one way to better understand some aspects of light dynamics is to look for simpler model operators which are more amenable to analysis but retain certain features of the full operator. In solid state physics, one such operator is the Harper operator [Hof76], and the purpose of this section is to motivate a photonic analog.
Let us consider the situation where a non-gyroscopic PhC is perturbed on the macroscopic level, i.e. we replace the periodic material weights \( w = (\epsilon, \mu) \) by \( w(\lambda) = (\epsilon_\lambda, \mu_\lambda) \) where these perturbed material weights

\[
\epsilon_\lambda(x) = \tau_\epsilon^{-2}(\lambda x) \epsilon(x), \\
\mu_\lambda(x) = \tau_\mu^{-2}(\lambda x) \mu(x),
\]

are modulated by bounded, strictly positive functions \( \tau_\epsilon \) and \( \tau_\mu \) whose inverses are also bounded. This type of perturbation has been studied theoretically \([RH08; EG13; DL14a]\) and models effects such as uneven thermal \([DWN+11; DLT+04]\) or uneven strain tuning \([WYR+04]\).

Quite naturally, the first task in the study of the perturbed Maxwell operator \( M_\lambda = M_w(\lambda) \) is to derive effective dynamics, i.e. to relate the perturbed to the unperturbed dynamics if one knows something about the initial states. Here, the states one considers are associated to a relevant family of frequency bands which is separated by a local gap from the others to prevent band transition. For instance, the bands \( \{\omega_\pm(k)\} \) or \( \{\omega_n(k), \omega_{n+}(k)\} \). However, we do allow band intersections within the family of relevant bands.

For the Bloch electron, the analogous situation in quantum mechanics, this is a very well-studied problem \([PST02]\). One type of effective dynamics are semiclassical dynamics: here, the band energy enters the Hamilton function, but the dynamical equations also contain a topological contribution in the form of the Berry curvature which acts as a pseudomagnetic field. Such semiclassical equations of motion, ray optics equations, have been proposed for PhCs by Raghu and Haldane \([RH08]\) and derived in \([OMN06; EG13]\). However, Real states can never be supported by single frequency bands so even in the simplest physically relevant situation, one has to work with a conjugate pair of bands \( \{\omega_\pm(k)\} = \{\omega(k), -\omega(-k)\} \). Then the single-band effective dynamics needs to be augmented by an analysis of an interband term (cf. the discussion in Section 6 of \([DL14a]\)).

So instead, let us pursue a different, complementary strategy to find effective dynamics in the twin-band case: here, one approximates \( e^{-itM_\lambda} \) on the subspace \( \text{ran} \Pi_\lambda \) defined in terms of the superadiabatic projection \( \Pi_\lambda = \Pi_0 + \mathcal{O}(\lambda) \) \([Nen91; PST02]\). The leading-order term \( \Pi_0 \) is unitarily equivalent to the family of the projections \( \sum_{j=\pm} |\varphi_j(k)\rangle \langle \varphi_j(k)| \) onto the eigenspaces of \( \omega_\pm \). Effective dynamics now means that there exists an effective Maxwell operator \( M_{\text{eff}} \) and a unitary \( U_\lambda \) such that

\[
\left( e^{-itM_\lambda} - U_\lambda^* e^{-itM_{\text{eff}}} U_\lambda \right) \Pi_\lambda = \mathcal{O}(\lambda^n)
\]

holds for some \( n \). This scheme has recently been implemented rigorously for photonic crystals \([DL14a]\), and \( U_\lambda, \Pi_\lambda \) and \( M_{\text{eff}} \) have been constructed order-by-order in \( \lambda \) via explicit recursion relations. The role of the unitary \( U_\lambda \) is to map the problem onto a simpler reference Hilbert space which in this case is \( L^2(\mathbb{B}) \otimes \mathbb{C}^N \) where \( \mathbb{B} \) is the Brillouin zone and in our case \( N = 2 \) since we are dealing with two non-degenerate bands.
The leading-order of $M_{\text{eff}}$ has been computed in [DL14a] for Bloch bands which individually carry zero Chern charge, and $M_{\text{eff}}$ is the “quantization” of

$$M_{\text{eff}}(r,k) = \tau(r) \begin{pmatrix} \omega(k) & 0 \\ 0 & -\omega(-k) \end{pmatrix}.$$ 

This is a matrix-valued function depending on macroscopic position $r$ and crystal momentum $k$, and involves the perturbation via the function $\tau(r) = \tau_\epsilon(r) \tau_\mu(r)$. After replacing $r$ with $i \lambda \nabla_k$ and $k$ with multiplication with $k$, the resulting Maxwell-Harper operator

$$M_{\text{eff}} = \frac{\tau(i \lambda \nabla_k)}{2} \begin{pmatrix} \omega(k) & 0 \\ 0 & -\omega(-k) \end{pmatrix} + \text{h.c.} \tag{5.1}$$

is the analog of “Peierls substitution” for PhCs.

One way to further analyze this operator is to assume $\tau$ is periodic on the macroscopic level; for instance, one can think of a finite sample of size $L = L_1 e_1, L_2 e_2, L_3 e_3$ where the $L_j$ are all positive, large integers, and we impose periodic boundary conditions. This gives rise to a lattice $\Gamma_L$ and a dual lattice $\Gamma^*_L$, and we can expand the modulation

$$\tau(r) = \sum_{\gamma \in \Gamma^*_L} \hat{\tau}(\gamma^*) e^{i \gamma^* \cdot r}$$

and the frequency band function

$$\omega(k) = \sum_{\gamma \in \Gamma} \hat{\omega}(\gamma) e^{i k \cdot \gamma}$$

in terms of the Fourier coefficients $\hat{\tau}(\gamma^*)$ and $\hat{\omega}(\gamma)$. The operator $M_{\text{eff}}$ can be expressed algebraically in terms of

$$(S_j \psi)(k) = e^{i k j} \psi(k), \quad (T_j \psi)(k) = \psi(k + \frac{\lambda}{L_j} e_j^*) = e^{i \frac{\lambda}{L_j} k j} \psi(k).$$

These two unitary operators are shifts in real and reciprocal space which satisfy the following commutation relations:

$$T_j S_n = e^{i \frac{\lambda}{L_j} \delta_{jn}} S_n T_j, \quad [T_j, T_n] = 0 = [S_j, S_n], \quad j, n = 1, 2, 3.$$

After a Fourier transform which maps $L^2(\Gamma^3)$ to $\ell^2(\Gamma)$, one obtains a multiband tight-binding model from (5.1) just as in condensed matter physics. Simplifying assumptions on the Fourier coefficients of $\omega$ and $\tau$ then lead to tight-binding models which can be analyzed efficiently and perhaps even explicitly.
These six operators generate a representation of a six-dimensional non-commutative torus on $L^2(\mathbb{T}^3)$ [VFG01, Chapter 12]. Let us denote the $C^*$-algebra generated by $S_j$ and $T_j$ on $L^2(\mathbb{T}^3)$ with $\mathcal{A}^{\mathbb{T}^3}(\lambda/L)$. We have shown that the effective models for the Maxwell dynamics in the twin bands case can be associated with a (diagonal) representative of the non-commutative torus $\mathcal{A}^{\mathbb{T}^3}(\lambda/L) \otimes \text{Mat}_C(2)$. This analogy allows us to apply all the well-known techniques for Harper operators to the Maxwell-Harper operator (5.1). For instance, one can expect to recover a Hofstadter’s butterfly-like spectrum [Hof76] which produces a splitting of the two topologically trivial bands $\omega_{\pm}$ into subbands which can carry a non-trivial topology. We stress that in this case the non-trivial effect is due only to an incommensurability between the perturbation parameter $\lambda$ and the lengths $L_j$ of the macroscopic lattice without any magnetic effect.

The operator (5.1) is just a particular example of a Maxwell-Harper operator; the fact that it is a diagonal element of $\mathcal{A}^{\mathbb{T}^3}(\lambda/L) \otimes \text{Mat}_C(2)$ can be linked to the topological triviality of $\omega_{\pm}$. However, in PhCs the presence of the PH symmetry does not imply the topological triviality of single bands, and the Bloch functions $\varphi_{\pm}(k)$ cannot be used to smoothly diagonalize $M_{\text{eff}}$. Instead, our arguments in Section 4 suggest to use Real and Imaginary part $\psi_{\text{Re}}$ and $\psi_{\text{Im}}$, and generally one obtains

$$M_{\text{eff}}(r,k) = \frac{\tau(r)}{2} \begin{pmatrix} \omega(k) - \omega(-k) & -i(\omega(k) + \omega(-k)) \\ i(\omega(k) + \omega(-k)) & \omega(k) - \omega(-k) \end{pmatrix}$$

which after the Peierls substitution produces a non diagonal element of $\mathcal{A}^{\mathbb{T}^3}(\lambda/L) \otimes \text{Mat}_C(2)$.

6 On the role of complex fields in gyrotropic PhCs

Our explanation for the absence of topological effects in non-gyroscopic PhCs hinged on the presence of the particle-hole symmetry and the assumption that the electromagnetic wave was purely real. However, the material weights in gyrotropic media are complex (such as is the case in [YCL99; WCJ+08; KRL+10; WLF+10], for instance), and the Maxwell equations are coupled PDEs with complex coefficients. So even if the initial states are real, the time-evolved fields acquire a non-zero imaginary part. Given how central the reality assumption was, the significance of truly complex electromagnetic fields needs to be explored. This is purely a problem of physics, because mathematically no fundamental obstacles arise in the analysis.

To the best of our knowledge this particular problem has seen very little attention in the literature. The best reference we have been able to track down is [Ber82] which covers the case of constant permittivity and permeability; its arguments extend readily to the present setting, but the author stops short of a complete physical interpretation of the complex nature of the plane wave solutions he gets. In standard textbooks (e.g. [Jac98]) complex electromagnetic fields are either discussed in the context of systems with friction or as a
convenient way to express solutions of the Maxwell equations in terms of complex plane waves rather than sin and cos. Neither one of these qualifications applies: In systems with friction or amplification, the eigenvalues of $\epsilon(x)$ and $\mu(x)$ need to have non-zero imaginary parts. As long as the material weights are hermitian, the field energy (2.6) is conserved because the Maxwell operator is selfadjoint.

Essentially, we see two ways to interpret complex electromagnetic waves:

(1) One takes the real part of the complex wave.

(2) One accepts the complex nature of the waves and that only real-valued quantities such as field intensities and the Poynting vector are measured in experiment.

The problem of strategy (1) is the interpretation of the imaginary part: where does the associated field energy go? And more importantly, our arguments from Section 4 show the absence of topological effects for states of the form $\text{Re}(E, H) = C\text{Re}(E, H)$. Clearly, this interpretation yields testable hypothesis that are incompatible with experiment (topological effects in PhCs have been observed [WCJ+08]).

The second interpretation is consistent with experiment, because it allows for topological effects. Electrodynamics in matter is an effective theory that is obtained after a suitable coarse graining procedure and holds only for electromagnetic waves whose in vacuo wavelength is large compared to the size of the constituents of the PhC (e.g. the size of split-ring resonators). So what is really measured in experiment? Observables in this context are real-valued functions in the fields such as the field intensities $|E(t, x)|^2$ and $|H(t, x)|^2$, and the Poynting vector

$$S = \text{Re} \, \mathbf{E} \times \mathbf{H}. \quad (6.1)$$

The definition of this vector stems from energy conservation (\cite[equation (38)]{Ber82}), namely if

$$U_\mathcal{E}(t, x) = \frac{1}{2} \left( E(t, x) \cdot \epsilon(x) E(t, x) + H(t, x) \cdot \mu(x) H(t, x) \right)$$

denotes the energy density, then $S$ satisfies the conservation law

$$\frac{\partial}{\partial t} U_\mathcal{E} + \nabla_x \cdot S = 0.$$

Lastly, how are gyrotrropic media different? After all, our arguments show that there is nothing mathematically wrong with having complex electromagnetic waves if all that counts is the propagation field intensity.
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