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Notes on the algebraic structure of wave equations

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There are many examples of wave equations in the physical sciences, characterized by oscillating solutions that propagate through space and time while, in lossless media, conserving energy. Examples include the scalar wave equation (e.g. pressure waves in a gas), Maxwell's equations (electromagnetism), Schrödinger's equation (quantum mechanics), elastic vibrations, and so on. From an algebraic perspective, all of these share certain common features. They can *all* be written abstractly in a form

$$\frac{\partial \mathbf{w}}{\partial t} = \hat{D} \mathbf{w} + \mathbf{s} \quad (1)$$

where $\mathbf{w}(\mathbf{x}, t)$ is some vector-field *wave function* characterizing the solutions (e.g. a 6-component electric+magnetic field in electromagnetism), \hat{D} is some *linear operator* (using the “hat” notation from quantum mechanics to denote linear operators), neglecting nonlinear effects, and $\mathbf{s}(\mathbf{x}, t)$ is some source term. The key property of \hat{D} for a wave equation is that it is *anti-Hermitian*, as opposed to a parabolic equation (e.g. a diffusion equation) where \hat{D} is Hermitian and negative semi-definite. From this anti-Hermitian property follow familiar features of wave equations, such as oscillating/propagating solutions and conservation of energy. In many cases, we will set $\mathbf{s} = 0$ and focus on the source-free behavior.

In the following note, we first derive some general properties of eq. (1) from the characteristics of \hat{D} , and then give examples of physical wave equations that can be written in this form and have these characteristics.

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1 General properties of wave equations

In lossless media, \hat{D} turns out to be an *anti-Hermitian* operator under some inner product $(\mathbf{w}, \mathbf{w}')$ between any two fields $\mathbf{w}(\mathbf{x}, t)$ and $\mathbf{w}'(\mathbf{x}, t)$ at a given time t . This means that $(\mathbf{w}, \hat{D}\mathbf{w}') = -(\hat{D}\mathbf{w}, \mathbf{w}')$ for any \mathbf{w}, \mathbf{w}' : \hat{D} flips sign when it moves from one side to the other of an inner product. This is proven below for several common wave equations. Formally, $\hat{D}^\dagger = -\hat{D}$, where \dagger is the adjoint: for any operator \hat{A} , $(\mathbf{w}, \hat{A}\mathbf{w}') = (\hat{A}^\dagger\mathbf{w}, \mathbf{w}')$ by definition of \hat{A}^\dagger .

The anti-Hermitian property of \hat{D} immediately leads to many useful consequences, and in particular the features that make the equation “wave-like:”

1.1 Harmonic modes and Hermitian eigenproblems

First, we can write down an *eigen-equation* for the *harmonic-mode* solutions $\mathbf{w}(\mathbf{x}, t) = \mathbf{W}(\mathbf{x})e^{-i\omega t}$, assuming \hat{D} is linear and time-invariant. Substituting $\mathbf{W}(\mathbf{x})e^{-i\omega t}$ into eq. (1) for the source-free $\mathbf{s} = 0$ case, we obtain:

$$\omega\mathbf{W} = i\hat{D}\mathbf{W}, \tag{2}$$

which is a *Hermitian* eigenproblem: if \hat{D} is anti-Hermitian, then $i\hat{D}$ is Hermitian. It then follows that the eigenvalues ω are real and that solutions \mathbf{W} can be chosen orthogonal. Notice that the real eigenvalues ω corresponds directly to our assumption that the medium has no dissipation (or gain)—if ω were complex, waves would exponentially decay (or grow), but instead they oscillate forever in time. For any reasonable physical problem, it also follows that the eigenmodes are a *complete basis* for all \mathbf{w} , so they completely characterize all solutions.¹

1.2 Planewave solutions

Second, the most familiar feature of wave equations is the existence of not just oscillation in *time* (real ω), but oscillation in *space* as well. In particular, with a wave equation

¹Technically, we require \hat{D} or its inverse to be *compact*, which is true as long as we have a reasonable decaying Green's function [1]. This is almost always true for physical wave problems, but functional analysts love to come up with pathological exceptions to this rule.

one immediately thinks of sinusoidal *planewave* solutions $\sim e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$ for some real *wave vector* \mathbf{k} . These solutions arise in *any* equation of the anti-Hermitian form (1) that additionally has *translational symmetry* (the medium is *homogeneous*).

Intuitively, translational symmetry means that \hat{D} is the same at different points in space. Formally, we can make this precise by defining a *translation operator* $\hat{T}_{\mathbf{d}}$ that takes a function $\mathbf{w}(\mathbf{x}, t)$ and translates it in space by a displacement \mathbf{d} :

$$\hat{T}_{\mathbf{d}}\mathbf{w}(\mathbf{x}, t) = \mathbf{w}(\mathbf{x} - \mathbf{d}, t).$$

When we say that \hat{D} has translational symmetry, we mean that \hat{D} is the same if we first translate by some \mathbf{d} , then operate \hat{D} , then translate back: $\hat{D} = \hat{T}_{\mathbf{d}}^{-1}\hat{D}\hat{T}_{\mathbf{d}}$, or equivalently \hat{D} *commutes* with $\hat{T}_{\mathbf{d}}$:

$$\hat{D}\hat{T}_{\mathbf{d}} = \hat{T}_{\mathbf{d}}\hat{D}$$

for *all* displacements \mathbf{d} . When one has commuting operators, however, one can choose simultaneous eigenvectors of both operators [2]. That means that the eigenvectors $\hat{W}(\mathbf{x})$ of $i\hat{D}$ (and \hat{D}) can be written in the form of eigenfunctions of $\hat{T}_{\mathbf{d}}$, which are exponential functions $e^{i\mathbf{k}\cdot\mathbf{x}}$ for some \mathbf{k} :

$$\mathbf{w}(\mathbf{x}, t) = \mathbf{W}(\mathbf{x})e^{-i\omega t} = \mathbf{W}_0e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} \quad (3)$$

for some constant vector \mathbf{W}_0 (depending on \mathbf{k} and ω) determined by \hat{D} . The wave vector \mathbf{k} must be real if we require our states to be bounded for all \mathbf{x} (not exponentially growing in any direction).² For each \mathbf{k} , there will be a discrete set of eigenfrequencies $\omega_n(\mathbf{k})$, called the *dispersion relation* or the *band structure* of the medium.

Let us also mention two generalizations, both of which follow from the broader viewpoint of *group representation theory* [3, 4]. First, the existence of planewave solutions can be thought of as a consequence of group theory. The symmetry operators that commute with \hat{D} form the *symmetry group* (or *space group*) of the problem (where the group operation is simply composition), and it can be shown that the eigenfunctions of \hat{D} can be chosen to transform as *irreducible representations* of the symmetry group. For the translation group $\{\hat{T}_{\mathbf{d}} \mid \mathbf{d} \in \mathbb{R}^3\}$, the irreducible representations are the exponential functions $\{e^{-i\mathbf{k}\cdot\mathbf{d}}\}$, but more complicated and interesting representations arise when one includes rotations and other symmetries. Second, in order to get wave solutions, one need not require \hat{D} to commute with $\hat{T}_{\mathbf{d}}$ for *all* \mathbf{d} . It is sufficient to require commutation for $\mathbf{d} = \mathbf{R} = n_1\mathbf{R}_1 + n_2\mathbf{R}_2 + n_3\mathbf{R}_3$ on a discrete periodic *lattice* \mathbf{R} with *primitive lattice vectors* \mathbf{R}_ℓ (and any $n_\ell \in \mathbb{Z}$): \hat{D} is *periodic*, with *discrete* translational symmetry. In this case, one obtains the *Bloch-Floquet theorem* (most famous in solid-state physics): the eigenfunctions \mathbf{W} can be chosen in the form of a plane

²Complex \mathbf{k} solutions are called *evanescent waves*, and can appear if \hat{D} is only translationally invariant over a finite region (e.g. if the medium is piecewise-constant). Even the real \mathbf{k} solutions are a bit weird because they are not normalizable: $\|e^{i\mathbf{k}\cdot\mathbf{x}}\|^2$ is not finite! By admitting such solutions, we are technically employing a “rigged” Hilbert space, which requires a bit of care but is not a major problem. Alternatively, we can put the whole system in a finite $L \times L \times L$ box with periodic boundary conditions, in which case the components of \mathbf{k} are restricted to discrete multiples of $2\pi/L$, and take the limit $L \rightarrow \infty$ at the end of the day.

wave multiplied by a periodic *Bloch envelope*. More explicitly, one has *Bloch wave* solutions:

$$\mathbf{w}(\mathbf{x}, t) = \mathbf{W}_{\mathbf{k},n}(\mathbf{x})e^{i[\mathbf{k}\cdot\mathbf{x}-\omega_n(\mathbf{k})t]}, \quad (4)$$

where $\mathbf{W}_{\mathbf{k},n}(\mathbf{x})$ is a periodic function (invariant under translation by any \mathbf{R} in the lattice) satisfying the Hermitian eigenproblem:

$$\omega_n(\mathbf{k})\mathbf{W}_{\mathbf{k},n} = ie^{-i\mathbf{k}\cdot\mathbf{x}}\hat{D}e^{i\mathbf{k}\cdot\mathbf{x}}\mathbf{W}_{\mathbf{k},n}.$$

The planewave case (3) [*continuous* translational symmetry] is simply the special case of the Bloch wave (4) [*discrete* translational symmetry] in the limit where the lattice vectors become infinitesimal ($|\mathbf{R}_\ell| \rightarrow 0$).

1.3 Time evolution and conservation of energy

Third, we obtain *conservation of energy* in the absence of sources ($\mathbf{s} = 0$), where we define the “energy” of a field \mathbf{w} as its norm $\|\mathbf{w}\|^2 = (\mathbf{w}, \mathbf{w})$. The proof that $\|\mathbf{w}\|^2$ is conserved for $\mathbf{s} = 0$ (sources would add or remove energy) is elementary, given an anti-Hermitian \hat{D} :

$$\frac{\partial\|\mathbf{w}\|^2}{\partial t} = \frac{\partial}{\partial t}(\mathbf{w}, \mathbf{w}) = (\dot{\mathbf{w}}, \mathbf{w}) + (\mathbf{w}, \dot{\mathbf{w}}) = (\hat{D}\mathbf{w}, \mathbf{w}) + (\mathbf{w}, \hat{D}\mathbf{w}) = (\hat{D}\mathbf{w}, \mathbf{w}) - (\hat{D}\mathbf{w}, \mathbf{w}) = 0.$$

This works even if \hat{D} is time-dependent, which may seem surprising: if you take a wave equation and “shake it” by varying \hat{D} rapidly in time, you might think you could add energy to the system. But no: a time-varying \hat{D} can alter the *frequency* of the solution (which is not conserved in a time-varying problem), but not the *energy*. However, this is not the whole story, because \hat{D} is not the only possible source of time-dependent behavior: the definition of our *inner product* $(\mathbf{w}, \mathbf{w}')$ can depend on t as well. In fact, we will see that this is often possible for physical systems such as Maxwell’s equations or even the scalar wave equation. In particular, our inner product is often of the form $(\mathbf{w}, \mathbf{w}') = (\mathbf{w}, \hat{P}\mathbf{w}')_0$, where $(\cdot, \cdot)_0$ denotes an inner product independent of time and \hat{P} is some positive-definite Hermitian operator depending on the wave medium, which may depend on time. In this case, when taking the time derivative of $\|\mathbf{w}\|^2$, we also get a term $(\mathbf{w}, \frac{\partial\hat{P}}{\partial t}\mathbf{w})_0$, which is not in general zero. So, a *time-varying medium* can break conservation of energy if the time variation *changes the norm*.

If \hat{D} is time-independent, we can easily write down the explicit solution of the initial-value problem. In this case eq. (1) for $\mathbf{s} = 0$ is solved formally by the operator exponential:

$$\mathbf{w}(\mathbf{x}, t) = e^{\hat{D}t}\mathbf{w}(\mathbf{x}, 0) = \hat{U}_t\mathbf{w}(\mathbf{x}, 0)$$

for an initial condition $\mathbf{w}(\mathbf{x}, 0)$ and a *time-evolution operator* $\hat{U}_t = e^{\hat{D}t}$. Because \hat{D} is anti-Hermitian, it flips sign when it switches sides in an inner product, and hence \hat{U}_t changes from $\hat{U}_t = e^{\hat{D}t}$ to $\hat{U}_t^\dagger = e^{-\hat{D}t} = \hat{U}_t^{-1} = \hat{U}_{-t}$. This means that \hat{U}_t is a *unitary* operator, and hence

$$\left\|\hat{U}_t\mathbf{w}\right\|^2 = (\hat{U}_t\mathbf{w}, \hat{U}_t\mathbf{w}) = (\hat{U}_t^{-1}\hat{U}_t\mathbf{w}, \mathbf{w}) = \|\mathbf{w}\|^2.$$

Thus, $\|\mathbf{w}\|^2$ does not change as the field evolves in time: energy is conserved!

1.4 Off-diagonal block form and reduced-rank eigenproblems

There is another variant on the eigenequation (2) $\omega \mathbf{W} = i\hat{D}\mathbf{W}$: if we operate $i\hat{D}$ again on both sides, we get $\omega^2 \mathbf{W} = -\hat{D}^2 \mathbf{W}$, where $-\hat{D}^2$ is automatically Hermitian and positive semi-definite. Why would we want to do this? The main reason is that \hat{D} often (not always) has a special block form:

$$\hat{D} = \begin{pmatrix} & \hat{D}_2 \\ \hat{D}_1 & \end{pmatrix}, \quad (5)$$

for some operators \hat{D}_1 and \hat{D}_2 , in which case \hat{D}^2 is *block diagonal*:

$$\hat{D}^2 = \begin{pmatrix} \hat{D}_2 \hat{D}_1 & 0 \\ 0 & \hat{D}_1 \hat{D}_2 \end{pmatrix}.$$

This means that the $\omega^2 \mathbf{W} = -\hat{D}^2 \mathbf{W}$ problem breaks into two *lower-dimensional* eigenproblems with operators $-\hat{D}_1 \hat{D}_2$ and $-\hat{D}_2 \hat{D}_1$. In particular, let us break our solution \mathbf{w} into two pieces:

$$\mathbf{w} = \begin{pmatrix} \mathbf{w}_1 \\ \mathbf{w}_2 \end{pmatrix}$$

where \hat{D}_k operates on \mathbf{w}_k , and suppose that our inner product also divides additively between these two pieces:

$$(\mathbf{w}, \mathbf{w}') = (\mathbf{w}_1, \mathbf{w}'_1)_1 + (\mathbf{w}_2, \mathbf{w}'_2)_2$$

in terms of some lower-dimensional inner products $(\cdot, \cdot)_1$ and $(\cdot, \cdot)_2$. In this case, from the fact that $-\hat{D}^2$ is Hermitian positive semi-definite under (\cdot, \cdot) , it immediately follows that $-\hat{D}_2 \hat{D}_1$ is Hermitian positive semi-definite under $(\cdot, \cdot)_1$ and $-\hat{D}_1 \hat{D}_2$ is Hermitian positive semi-definite under $(\cdot, \cdot)_2$. (To prove this, just write down the Hermitian positive-semidefinite property of $-\hat{D}^2$ for $\mathbf{w}_k = 0$ with $k = 1, 2$.) We therefore have obtained two smaller Hermitian positive semi-definite eigenproblems

$$-\hat{D}_2 \hat{D}_1 \mathbf{W}_1 = \omega^2 \mathbf{W}_1, \quad (6)$$

$$-\hat{D}_1 \hat{D}_2 \mathbf{W}_2 = \omega^2 \mathbf{W}_2, \quad (7)$$

again with real ω solutions and orthogonality relations on the \mathbf{W}_k .³

Moreover, each of these has to give *all* of the eigenfrequencies ω . Every eigenfunction of \hat{D} must obviously be an eigenfunction of \hat{D}^2 , and the converse is also true: given an eigenvector \mathbf{W}_1 of eq. (6) with eigenvalue ω^2 , to get an eigenvector \mathbf{W} of \hat{D} with eigenvalue ω we just set

$$\mathbf{W}_2 = \frac{i}{\omega} \hat{D}_1 \mathbf{W}_1. \quad (8)$$

³The fact that they are positive semi-definite (and often positive-definite, since it is typically possible to exclude the $\omega = 0$ solutions) is especially advantageous for numerical methods. Some of the best iterative eigensolver methods are restricted to positive-definite Hermitian problems, for example [5].

This formula looks a bit suspicious in the case where $\omega = 0$: the *static* (non-oscillatory) solutions. For these (usually less-interesting) static solutions, the \mathbf{W}_1 and \mathbf{W}_2 eigenproblems decouple from one another and we can just set $\mathbf{W}_2 = 0$ in \mathbf{W} . Similarly, if we solve for an eigenvector \mathbf{W}_2 of eq. (7), we can construct \mathbf{W} via $\mathbf{W}_1 = i\hat{D}_2\mathbf{W}_2/\omega$ for $\omega \neq 0$ or set $\mathbf{W}_1 = 0$ for $\omega = 0$.

We lost the sign of ω by squaring it (which is precisely why we can solve an eigenproblem of “half” the size), but this doesn’t matter: $\omega = \pm\sqrt{\omega^2}$ both yield eigen-solutions \mathbf{W} by (8). Therefore, in problems of the block form (5), the eigenvalues ω *always* come in positive/negative pairs. In the common case where \hat{D}_1 and \hat{D}_2 are purely *real*, the eigenvectors \mathbf{W}_1 (or \mathbf{W}_2) can also be chosen real, we can therefore obtain real solutions \mathbf{w} by adding the $+\omega$ and $-\omega$ eigenfunctions (which are complex conjugates).

1.5 Harmonic sources and reciprocity

The most important kind of source \mathbf{s} is a *harmonic* source

$$\mathbf{s}(\mathbf{x}, t) = \mathbf{S}(\mathbf{x})e^{-i\omega t}.$$

In this case, we are looking for the *steady-state* response $\mathbf{w} = \mathbf{W}(\mathbf{x})e^{-i\omega t}$. Substituting these into eq. (1) problem of solving for $\mathbf{W}(\mathbf{x})$ is now in the form of an ordinary linear equation, rather than an eigenproblem:

$$(i\hat{D} - \omega) \mathbf{W} = \hat{O}\mathbf{W} = -i\mathbf{S}.$$

Notice that the operator $\hat{O} = i\hat{D} - \omega$ on the left-hand side is Hermitian. Suppose that we solve the equation twice, with sources $\mathbf{S}^{(1)}$ and $\mathbf{S}^{(2)}$ to get solutions $\mathbf{W}^{(1)}$ and $\mathbf{W}^{(2)}$. Then, the Hermitian property means that we obtain the following identity for the inner product:

$$(\mathbf{W}^{(1)}, \mathbf{S}^{(2)}) = (\mathbf{W}^{(1)}, i\hat{O}\mathbf{W}^{(2)}) = (-i\hat{O}\mathbf{W}^{(1)}, \mathbf{W}^{(2)}) = -(\mathbf{S}^{(1)}, \mathbf{W}^{(2)}).$$

This is *almost* the same as a very well known property of wave equations, known as *reciprocity*. The reason it is only *almost* the same is that reciprocity relations normally use an *unconjugated* “inner product,” assuming \hat{O} is not only Hermitian but real (or complex-symmetric). This gets rid of the minus sign on the right-hand side, for one thing. It also only requires $i\hat{D}$ to be complex-symmetric (Hermitian under an unconjugated inner product) rather than Hermitian, which allows reciprocity to apply even to systems with dissipation. (It also simplifies some technical difficulties regarding the boundary conditions at infinity.) See e.g. Ref. [6].

What if \hat{O} is not real or complex-symmetric, e.g. in the common case where \hat{D} is real-antisymmetric? Can we still have reciprocity with an unconjugated inner product? In this case, we can often instead express reciprocity using the block form (5), since in that case the operator is real-symmetric if \hat{D} is real, as described below.

Just as for the eigenproblem, it is common when we have the block form (5) of \hat{D} to break the problem into a smaller linear equation for \mathbf{W}_1 or \mathbf{W}_2 , similarly subdividing

$\mathbf{S} = (\mathbf{S}_1; \mathbf{S}_2)$. For example, the equation for \mathbf{W}_1 is

$$(-\hat{D}_2\hat{D}_1 - \omega^2)\mathbf{W}_1 = -i\omega\mathbf{S}_1 + \hat{D}_2\mathbf{S}_2. \quad (9)$$

For example, in the case of the scalar wave equation below, this equation becomes a inhomogeneous scalar Helmholtz equation. Again, notice that the operator $-\hat{D}_2\hat{D}_1 - \omega^2$ on the left-hand side is Hermitian. In fact, it is often purely real-symmetric (or complex-symmetric in a system with dissipation), which allows us to derive reciprocity using an unconjugated inner product as described above.

2 The scalar wave equation

There are many formulations of waves and wave equations in the physical sciences, but the prototypical example is the (source-free) *scalar wave equation*:

$$\nabla \cdot (a\nabla u) = \frac{1}{b} \frac{\partial^2 u}{\partial t^2} = \frac{\ddot{u}}{b} \quad (10)$$

where $u(\mathbf{x}, t)$ is the scalar wave amplitude and $c = \sqrt{ab}$ is the phase velocity of the wave for some parameters $a(\mathbf{x})$ and $b(\mathbf{x})$ of the (possibly inhomogeneous) medium.⁴ This can be written in the form of eq. (1) by splitting into two first-order equations, in terms of u and a new vector variable \mathbf{v} satisfying $a\nabla u = \dot{\mathbf{v}}$ and $b\nabla \cdot \mathbf{v} = \dot{u}$:

$$\frac{\partial \mathbf{w}}{\partial t} = \frac{\partial}{\partial t} \begin{pmatrix} u \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} & b\nabla \cdot \\ a\nabla & \end{pmatrix} \begin{pmatrix} u \\ \mathbf{v} \end{pmatrix} = \hat{D}\mathbf{w}$$

for a 4×4 linear operator \hat{D} and a 4-component vector $\mathbf{w} = (u; \mathbf{v})$, in 3 spatial dimensions.

Next, we need to show that \hat{D} is anti-Hermitian, for the case of lossless media where a and b are real and positive. To do this, we must first define an inner product $(\mathbf{w}, \mathbf{w}')$ by the integral over all space:

$$(\mathbf{w}, \mathbf{w}') = \int [u^* (b^{-1}u') + \mathbf{v}^* (a^{-1}\mathbf{v}')] d^3\mathbf{x},$$

where $*$ denotes the complex conjugate (allowing complex \mathbf{w} for generality).

Now, in this inner product, it can easily be verified via integration by parts that:

$$(\mathbf{u}, \hat{D}\mathbf{u}') = \int [u^* \nabla \cdot \mathbf{v}' + \mathbf{v}^* \cdot \nabla u'] d^3\mathbf{x}, = \dots = -(\hat{D}\mathbf{u}, \mathbf{u}'),$$

which by definition means that \hat{D} is *anti-Hermitian*. All the other properties—conservation of energy, real eigenvalues, etcetera—then follow.

Also, note that the $-\hat{D}^2$ eigenproblem in this case gives us more-convenient smaller eigenproblems, as noted earlier: $-b\nabla \cdot (a\nabla u) = \omega^2 u$, and $-a\nabla (b\nabla \cdot \mathbf{v}) = \omega^2 \mathbf{v}$. (These may not look Hermitian, but remember our inner product.) And in the harmonic-source case, we get an operator $-\hat{D}_2\hat{D}_1 - \omega^2 = -b\nabla \cdot a\nabla - \omega^2$ when solving for u via (9)—for the common case $a = b = 1$, this is the scalar Helmholtz operator $-(\nabla^2 + \omega^2)$.

⁴More generally, a may be a 3×3 tensor in an anisotropic medium.

3 Maxwell's equations

Maxwell's equations, in terms of the electric field \mathbf{E} , magnetic field \mathbf{H} , dielectric permittivity ε and magnetic permeability μ , are:

$$\begin{aligned}\nabla \times \mathbf{E} &= -\frac{\partial(\mu\mathbf{H})}{\partial t} \\ \nabla \times \mathbf{H} &= \frac{\partial(\varepsilon\mathbf{E})}{\partial t} + \mathbf{J},\end{aligned}$$

where \mathbf{J} is a current source; $\mathbf{J} = 0$ in the source-free case. The other two Maxwell's equations $\nabla \cdot \varepsilon\mathbf{E} = 0$ and $\nabla \cdot \mu\mathbf{H} = 0$ express constraints on the fields (in the absence of free charge) that are preserved by the above two dynamical equations, and can thus be ignored for the purposes of this analysis (they are just constraints on the initial conditions). For simplicity, we restrict ourselves to the case where ε and μ do not depend on time: the materials may vary with position \mathbf{x} , but they are not moving or changing.⁵ ε and μ may also be 3×3 tensors rather than scalars, in an anisotropic medium, but we assume that they are Hermitian positive-definite in order to be a lossless and transparent medium. In this case, the equations can be written in the form of (1) via:

$$\frac{\partial \mathbf{w}}{\partial t} = \frac{\partial}{\partial t} \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} = \begin{pmatrix} \frac{1}{\varepsilon} \nabla \times & \\ -\frac{1}{\mu} \nabla \times & \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix} + \begin{pmatrix} -\mathbf{J}/\varepsilon \\ \mathbf{0} \end{pmatrix} = \hat{D}\mathbf{w} + \mathbf{s},$$

where \mathbf{w} here is a 6-component vector field.

To show that this \hat{D} is anti-Hermitian, we must again define an inner product by an integral over space at a fixed time:

$$(\mathbf{w}, \mathbf{w}') = \frac{1}{2} \int [\mathbf{E}^* \cdot (\varepsilon\mathbf{E}') + \mathbf{H}^* \cdot (\mu\mathbf{H}')] d^3\mathbf{x},$$

which is precisely the classical electromagnetic energy in the \mathbf{E} and \mathbf{H} fields (for non-dispersive materials) [7]!

Given this inner product, the rest is easy, given a single vector identity: for any vector fields \mathbf{F} and \mathbf{G} , $\nabla \cdot (\mathbf{F} \times \mathbf{G}) = \mathbf{G} \cdot (\nabla \times \mathbf{F}) - \mathbf{F} \cdot (\nabla \times \mathbf{G})$. This vector identity allows us to integrate $\nabla \times$ by parts easily: $\int \mathbf{F} \cdot (\nabla \times \mathbf{G}) = \int \mathbf{G} \cdot (\nabla \times \mathbf{F})$ plus a surface term (from the divergence theorem) that goes to zero assuming $\|\mathbf{F}\|$ and $\|\mathbf{G}\|$ are $< \infty$.

Now we can just plug in $(\mathbf{w}, \hat{D}\mathbf{w}')$ and integrate by parts:

$$\begin{aligned}(\mathbf{w}, \hat{D}\mathbf{w}') &= \frac{1}{2} \int [\mathbf{E}^* \cdot (\nabla \times \mathbf{H}') - \mathbf{H}^* \cdot (\nabla \times \mathbf{E}')] d^3\mathbf{x} \\ &= \frac{1}{2} \int [(\nabla \times \mathbf{E})^* \cdot \mathbf{H}' - (\nabla \times \mathbf{H})^* \cdot \mathbf{E}'] d^3\mathbf{x} = (-\hat{D}\mathbf{w}, \mathbf{w}').\end{aligned}$$

Thus, \hat{D} is Hermitian and conservation of energy, real ω , orthogonality, etcetera follow.

⁵One can get very interesting physics by including the possibility of time-varying materials!

Again, \hat{D} is in the block form (5), so the \hat{D}^2 eigenproblem simplifies into two separate Hermitian positive semi-definite eigenproblems for \mathbf{E} and \mathbf{H} :

$$\frac{1}{\varepsilon} \nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{E} \right) = \omega^2 \mathbf{E}, \quad (11)$$

$$\frac{1}{\mu} \nabla \times \left(\frac{1}{\varepsilon} \nabla \times \mathbf{H} \right) = \omega^2 \mathbf{H}. \quad (12)$$

These convenient formulations are a more common way to write the electromagnetic eigenproblem [8] than (2). Again, they may not look very Hermitian because of the $1/\varepsilon$ and $1/\mu$ terms multiplying on the left, but don't forget the ε and μ factors in our inner product, which makes these operators Hermitian.⁶ Therefore, for example, two different eigensolutions \mathbf{E}_1 and \mathbf{E}_2 are orthogonal under the inner product $(\mathbf{E}_1, \mathbf{E}_2)_{\mathbf{E}} = \int \mathbf{E}_1^* \cdot (\varepsilon \mathbf{E}_2) = 0$. Bloch's theorem (4) for this Hermitian eigenproblem in the case of periodic materials leads to *photonic crystals* [8].

Recall that something funny happens at $\omega = 0$, where \mathbf{E} and \mathbf{H} decouple. In this case, there are infinitely many $\omega = 0$ *static-charge* solutions with $\nabla \cdot \varepsilon \mathbf{E} \neq 0$ and/or $\nabla \cdot \mu \mathbf{H} \neq 0$. For $\omega \neq 0$, $\nabla \cdot \varepsilon \mathbf{E} = 0$ and $\nabla \cdot \mu \mathbf{H} = 0$ follow automatically from the equations $-i\omega \varepsilon \mathbf{E} = \nabla \times \mathbf{H}$ and $i\omega \mu \mathbf{H} = \nabla \times \mathbf{E}$. (These divergence equations are just Gauss' laws for the free electric and magnetic charge densities, respectively.)

In the case with a current source $\mathbf{J} \neq 0$, we can solve for \mathbf{E} via eq. (9), which here becomes:

$$\left(\frac{1}{\varepsilon} \nabla \times \frac{1}{\mu} \nabla \times -\omega^2 \right) \mathbf{E} = i\omega \mathbf{J}/\varepsilon,$$

or (multiplying both sides by ε)

$$\left(\nabla \times \frac{1}{\mu} \nabla \times -\omega^2 \varepsilon \right) \mathbf{E} = i\omega \mathbf{J}.$$

The operator on the left side is Hermitian in lossless media, or complex-symmetric in most dissipative materials where ε and μ are complex scalars. This gives rise to the well-known Rayleigh-Carson and Lorentz reciprocity relations [9, 6].

4 The one-way scalar wave equation

As a break from the complexity of Maxwell's equations, let's look at the source-free one-way scalar wave equation:

$$-c \frac{\partial u}{\partial x} = \frac{\partial u}{\partial t},$$

⁶Alternatively, if we defined inner products without the ε and μ , we could write it as a *generalized* Hermitian eigenproblem. For example, if we used the inner product $(\mathbf{E}, \mathbf{E}') = \int \mathbf{E}^* \cdot \mathbf{E}'$, we would write the generalized Hermitian eigenproblem $\nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{E} \right) = \omega^2 \varepsilon \mathbf{E}$. This gives the same result: for generalized Hermitian eigenproblems $\hat{A}u = \lambda \hat{B}u$, the orthogonality relation is $(u_1, \hat{B}u_2) = 0$ for distinct eigenvectors u_1 and u_2 . This formulation is often more convenient than having ε or μ factors "hidden" inside the inner product.

where $c(\mathbf{x}) > 0$ is the phase velocity. This is a *one-way* wave equation because, for $c = \text{constant}$, the solutions are functions $u(x, t) = f(x - ct)$ traveling in the $+x$ direction *only* with speed c .

This equation is *already* in our form (1), with $\hat{D} = -c\frac{\partial}{\partial x}$, which is obviously anti-Hermitian under the inner product

$$(u, u') = \int_{-\infty}^{\infty} \frac{u^* u'}{c} dx,$$

via elementary integration by parts. Hence energy is conserved, we have real eigenvalues, orthogonality, and all of that good stuff. We *don't* have the block form (5), which is not surprising: we can hardly split this trivial equation into two simpler ones.

5 The Schrödinger equation

Perhaps the most famous equation in form (1) is the Schrödinger equation of quantum mechanics:

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} \left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi,$$

for the wave function $\psi(\mathbf{x}, t)$ of a particle with mass m in a (real) potential $V(\mathbf{x})$. Famous, not so much because Schrödinger is more well known than, say, Maxwell's equations, but rather because the Schrödinger equation (unlike Maxwell) is commonly taught almost precisely in the abstract form (1) [2, 10], where the operator \hat{D} is given by

$$\hat{D} = -\frac{i}{\hbar} \hat{H} = -\frac{i}{\hbar} \left(-\frac{\hbar^2}{2m} \nabla^2 + V \right)$$

for the *Hamiltonian* operator \hat{H} . This is the equation where many students delve into abstract Hermitian operators and Hilbert spaces for the first time.

The fact that \hat{H} is Hermitian under the inner product $(\psi, \psi') = \int \psi^* \psi'$, and hence \hat{D} is anti-Hermitian, is well known (and easy to show via integration by parts). From this follow the familiar properties of the Schrödinger equation. The eigenvalues ω are interpreted as the energies $E = \hbar\omega$, which are real (like any quantum observable), and the eigenstates ψ are orthogonal. Conservation of “energy” here means that $\int |\psi|^2$ is a constant over time, and this is interpreted in quantum mechanics as the conservation of probability.

Again, we *don't* have a block form (5) for the Schrödinger problem, nor do we want it. In this case, the operator \hat{D} is *not* real, and we *do* distinguish positive and negative ω (which give very different energies E !). We want to stick with the full eigenproblem $\hat{D}\psi = \omega\psi$, or equivalently $\hat{H}\psi = E\psi$, thank you very much. Bloch's theorem (4) for this Hermitian eigenproblem in the case of a periodic potential V leads to the field of *solid-state physics* for crystalline materials [11, 12].

6 Elastic vibrations in linear solids

One of the more complicated wave equations is that of elastic (acoustic) waves in solid media, for which there are three kinds of vibrating waves: longitudinal (pressure/compression) waves and two orthogonal transverse (shear) waves. All of these solutions are characterized by the displacement vector $\mathbf{u}(\mathbf{x}, t)$, which describes the displacement \mathbf{u} of the point \mathbf{x} in the solid at time t .

In the linear regime, an isotropic elastic medium is characterized by its density ρ and the Lamé elastic constants μ and λ : μ is the shear modulus and $\lambda = K - \frac{2}{3}\mu$, where K is the bulk modulus. All three of these quantities are functions of \mathbf{x} for an inhomogeneous medium. The displacement \mathbf{u} then satisfies the Lamé-Navier equation [13, 14]:

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla(\lambda \nabla \cdot \mathbf{u}) + \nabla \cdot [\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{f}, \quad (13)$$

where $\mathbf{f}(\mathbf{x}, t)$ is a source term (an external force density). This notation requires a bit of explanation. By $\nabla \mathbf{u}$, we mean the rank-2 tensor (3×3 matrix) with (m, n) th entry $\partial u_m / \partial x_n$ (that is, its rows are the gradients of each component of \mathbf{u}), and $(\nabla \mathbf{u})^T$ is the transpose of this tensor. By the divergence $\nabla \cdot$ of such a tensor, we mean the vector formed by taking the divergence of each *column* of the tensor (exactly like the usual rule for taking the dot product of a vector with a 3×3 matrix).

Clearly, we must break eq. (13) into two first-order equations in order to cast it into our abstract form (1), but what variables should we choose? Here, we can be guided by the fact that we eventually want to obtain conservation of energy, so we can look at what determines the physical energy of a vibrating wave. The kinetic energy is obviously the integral of $\frac{1}{2} \rho |\mathbf{v}|^2$, where \mathbf{v} is the velocity $\dot{\mathbf{u}}$, so \mathbf{v} should be one of our variables. To get the potential energy, is convenient to first define the (symmetric) *strain tensor* ε [14]:

$$\varepsilon = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T), \quad (14)$$

which should look familiar because 2ε appears in eq. (13). In terms of ε , the potential energy density is then $\mu \text{tr}(\varepsilon^\dagger \varepsilon) + \lambda |\text{tr} \varepsilon|^2 / 2$, where \dagger is the conjugate-transpose (adjoint) [14]. Note also that $\text{tr} \varepsilon = \nabla \cdot \mathbf{u}$, by definition of ε .

Therefore, we should define our wave field \mathbf{w} as the 9-component $\mathbf{w} = (\mathbf{v}; \varepsilon)$, with an inner product

$$(\mathbf{w}, \mathbf{w}') = \frac{1}{2} \int [\rho \mathbf{v}^* \cdot \mathbf{v}' + 2\mu \text{tr}(\varepsilon^\dagger \varepsilon') + \lambda (\text{tr} \varepsilon)^* (\text{tr} \varepsilon')] d^3 \mathbf{x},$$

so that $\|\mathbf{w}\|^2$ is the physical energy. Now, in terms of \mathbf{v} and ε , our equations of motion must be:

$$\frac{\partial \mathbf{w}}{\partial t} = \frac{\partial}{\partial t} \begin{pmatrix} \mathbf{v} \\ \varepsilon \end{pmatrix} = \begin{pmatrix} \hat{D}_2 \\ \hat{D}_1 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \varepsilon \end{pmatrix} + \begin{pmatrix} \mathbf{f}/\rho \\ 0 \end{pmatrix} = \hat{D} \mathbf{w} + \mathbf{s},$$

with

$$\dot{\varepsilon} = \hat{D}_1 \mathbf{v} = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T), \quad (15)$$

$$\dot{\mathbf{v}} = \hat{D}_2 \varepsilon = \frac{1}{\rho} [\nabla(\lambda \operatorname{tr} \varepsilon) + 2\nabla \cdot (\mu \varepsilon)].$$

Now, we can check that \hat{D} is anti-Hermitian (assuming lossless materials, i.e. real λ and μ). For compactness, we will use the Einstein index notation that repeated indices are summed, e.g. $\mathbf{a} \cdot \mathbf{b} = a_n b_n$ with an implicit sum over n since it is repeated, and let ∂_k denote $\frac{\partial}{\partial x_k}$. Then, plugging in the definitions above and integrating by parts:

$$\begin{aligned} (\mathbf{w}, \hat{D}\mathbf{w}') &= \frac{1}{2} \int \left[\rho \mathbf{v}^* \cdot (\hat{D}_2 \varepsilon') + 2\mu \operatorname{tr}(\varepsilon^\dagger \hat{D}_1 \mathbf{v}') + \lambda (\operatorname{tr} \varepsilon)^* (\operatorname{tr} \hat{D}_1 \mathbf{v}') \right] d^3 \mathbf{x} \\ &= \frac{1}{2} \int \left[v_m^* (\partial_m \lambda \varepsilon'_{nn} + 2\partial_n \mu \varepsilon'_{nm}) + 2\mu \varepsilon_{mn}^* \partial_m v'_n + \lambda (\varepsilon_{mm})^* (\partial_n v'_n) \right] d^3 \mathbf{x} \\ &= \frac{-1}{2} \int \left[(\lambda \partial_m v_m)^* \varepsilon'_{nn} + (2\mu \partial_n v_m)^* \varepsilon_{nm} + (2\partial_m \mu \varepsilon_{mn})^* v'_n + (\partial_n \lambda \varepsilon_{mm})^* v'_n \right] d^3 \mathbf{x} \\ &= (\hat{D}\mathbf{w}, \mathbf{w}'). \end{aligned}$$

Note that we used the symmetry of ε to write $2 \operatorname{tr}(\varepsilon^\dagger \hat{D}_1 \mathbf{v}') = \varepsilon_{mn}^* \partial_m v'_n + \varepsilon_{mn}^* \partial_n v'_m = 2\varepsilon_{mn}^* \partial_m v'_n$.

We are done! After a bit of effort to define everything properly and prove the anti-Hermitian property of \hat{D} , we can again immediately quote all of the useful general properties of wave equations: oscillating solutions, planewaves in homogeneous media, conservation of energy, and so on!

6.1 Scalar pressure waves in a fluid or gas

For a fluid or gas, the shear modulus μ is zero—there are no transverse waves—and λ is just the bulk modulus. In this case, we can reduce the problem to a scalar wave equation in terms of the pressure $P = -\lambda \nabla \cdot \mathbf{u} = -\operatorname{tr} \varepsilon$. We obtain *precisely* the scalar wave equation (10) if we set $a = 1/\rho$, $b = \lambda$, $u = P$, and $\mathbf{v} = -\dot{\mathbf{u}}$ (the velocity, with a sign flip by the conventions defined in our scalar-wave section). The wave speed is $c = \sqrt{\lambda/\rho}$. Our “energy” in the scalar wave equation is again interpreted as (twice) the physical energy: the integral of (twice) the potential energy P^2/λ and (twice) the kinetic energy $\rho|\mathbf{v}|^2$.

6.2 Eigenequations and constraints

Again, we have the block form (5) of \hat{D} , so again we can write an eigenproblem for ω^2 by solving for harmonic \mathbf{v} or ε individually. Given a harmonic $\mathbf{u} = \mathbf{U}(\mathbf{x})e^{-i\omega t}$, the equation for \mathbf{U} just comes from the eigen-equation for $\mathbf{v} = -i\omega \mathbf{U}e^{-i\omega t}$, which is just the same as plugging a harmonic \mathbf{u} into our original equation (13):

$$\omega^2 \mathbf{U} = -\frac{1}{\rho} \left\{ \nabla(\lambda \nabla \cdot \mathbf{U}) + \nabla \cdot [\mu (\nabla \mathbf{U} + (\nabla \mathbf{U})^T)] \right\},$$

which again is a Hermitian positive semi-definite eigenproblem thanks to the factor of ρ in our inner product $(\mathbf{U}, \mathbf{U}') = \int \rho \mathbf{U}^* \cdot \mathbf{U}'$. (Alternatively, one obtains a generalized Hermitian eigenproblem for an inner product without ρ .) Bloch’s theorem (4) for this

Hermitian eigenproblem in the case of periodic materials leads to the study of *phononic crystals* [15].

We could also write the eigenequation in terms of ε , of course. Sometimes, ε is more convenient because of how boundary conditions are expressed in elastic problems [14]. However, in the case of ε we need to enforce the constraint

$$\nabla \times (\nabla \times \varepsilon)^T = 0, \quad (16)$$

which follows from the definition (14) of ε in terms of \mathbf{u} . Note that the curl of a tensor, here, is defined as the curl of each column of the tensor, so $\nabla \times (\nabla \times \varepsilon)^T$ means that we take the curl of every row and column of ε . This is zero because ε is defined as the sum of a tensor whose rows are gradients and its transpose, and the curl of a gradient is zero. The same constraint also follows from eq. (15) for $\omega \neq 0$, which is part of the eigenequation, but ε is decoupled from eq. (15) for $\omega = 0$ and in that case we need to impose (16) explicitly [14].

7 The scalar wave equation in space

Now, let's consider something a little different. We'll start with the scalar wave equation from above, $a\nabla u = \dot{\mathbf{v}}$ and $b\nabla \cdot \mathbf{v} = \dot{u}$, but instead of solving for u and \mathbf{v} as a function of time t , we'll solve the equations as a function of *space* for harmonic modes $u(\mathbf{x}, t) = U(\mathbf{x})e^{-i\omega t}$ and $\mathbf{v}(\mathbf{x}, t) = \mathbf{V}(\mathbf{x})e^{-i\omega t}$ with $\omega \neq 0$. In particular, we'll pick one direction, z , and look at propagation along the z direction. Plugging these harmonic modes into the scalar wave equations, and putting all of the $\partial/\partial z$ derivatives on the left-hand side, we obtain:

$$\frac{\partial \mathbf{w}}{\partial z} = \frac{\partial}{\partial z} \begin{pmatrix} U \\ V_z \end{pmatrix} = \begin{pmatrix} 0 & -\frac{i\omega}{b} + \nabla_t \cdot \frac{a}{i\omega} \nabla_t \\ \frac{-i\omega}{a} & 0 \end{pmatrix} \begin{pmatrix} U \\ V_z \end{pmatrix} = \hat{D}\mathbf{w},$$

where $\nabla_t = \hat{\mathbf{x}} \frac{\partial}{\partial x} + \hat{\mathbf{y}} \frac{\partial}{\partial y}$ denotes the “transverse” (xy) del operator, and we have eliminated the transverse components \mathbf{V}_t of \mathbf{V} via $-i\omega \mathbf{V}_t = a \nabla_t U$. This is again of the form of our abstract equation (1), with z replacing t ! But is this \hat{D} anti-Hermitian?

Let's define our “inner product” via an integral over the xy plane:

$$(\mathbf{w}, \mathbf{w}') = \int [U^* V'_z + U' V_z^*] d^2 \mathbf{x}. \quad (17)$$

This is actually *not a true inner product* by the strict definition, because it is not positive definite: it is possible for $\|\mathbf{w}\|^2 = (\mathbf{w}, \mathbf{w})$ to be non-positive for $\mathbf{w} \neq 0$. We'll have to live with the consequences of that later. But first, let's verify that $(\mathbf{w}, \hat{D}\mathbf{w}') = -(\hat{D}\mathbf{w}, \mathbf{w}')$ for real a and b , via integration by parts:

$$\begin{aligned} (\mathbf{w}, \hat{D}\mathbf{w}') &= \int \left[U^* \left(-\frac{i\omega}{b} U' \right) + U^* \nabla_t \cdot \frac{a}{i\omega} \nabla_t U' + \left(-\frac{i\omega}{a} V'_z \right) V_z^* \right] d^2 \mathbf{x} \\ &= - \int \left[\left(-\frac{i\omega}{b} U \right)^* U' + (\nabla_t \cdot \frac{a}{i\omega} \nabla_t U^*) U' + \left(-\frac{i\omega}{b} V_z \right)^* + V'_z \left(-\frac{i\omega}{a} V_z^* \right) \right] d^2 \mathbf{x} \\ &= -(\hat{D}\mathbf{w}, \mathbf{w}'). \end{aligned}$$

So \hat{D} is “anti-Hermitian,” but in a “fake” inner product. To figure out the consequences of this, we have to go back to our original abstract derivations and look carefully to see where (if at all) we relied on the positive-definite property of inner products.

Looking back at our proof, we see that we didn’t rely on positive-definiteness at all in our derivation of conservation of energy; we just took the derivative of (\mathbf{w}, \mathbf{w}) . So, “energy” is conserved in *space*. What does that mean? Equation (17) can be interpreted as an integral of a time-average *energy flux* through the xy plane at z . Conservation of energy means that, in the absence of sources, with a steady-state (harmonic) solution, energy cannot be building up or decaying at any z .

What about the Hermitian eigenproblem? What is the eigenproblem? We already have time-harmonic solutions. We can set up an eigenproblem in z only when the problem (i.e., a and b) is z -invariant (analogous to the time-invariance required for time-harmonic modes).⁷ In a z -invariant problem, the z direction is separable and we can look for solutions of the form $\mathbf{w}(x, y, z) = \mathbf{W}(x, y)e^{i\beta z}$, where β is a *propagation constant*. Such solutions satisfy

$$i\hat{D}\mathbf{W} = \beta\mathbf{W},$$

which is a Hermitian eigenproblem but in our non-positive norm. Now, if one goes back to the derivation of real eigenvalues for Hermitian eigenproblems, something goes wrong: the eigenvalue β is only real if $(\mathbf{W}, \mathbf{W}) \neq 0$.

This, however is a useful and important result, once we recall that (\mathbf{W}, \mathbf{W}) is the “energy flux” in the z direction. Modes with real β are called *propagating modes*, and they have non-zero flux: propagating modes *transport energy* since $(\mathbf{W}, \mathbf{W}) \neq 0$ for a typical real- β mode.⁸ Modes with complex (most often, purely imaginary) β are called *evanescent modes*, and they do *not* transport energy since $(\mathbf{W}, \mathbf{W}) = 0$ for them.

What about orthogonality? Again, going back to the derivation of orthogonality for Hermitian eigenproblems, and not assuming the eigenvalues are real (since they aren’t for evanescent modes). The orthogonality condition follows from the equation $[\beta^* - \beta'] \cdot (\mathbf{W}, \mathbf{W}') = 0$ for eigensolutions \mathbf{W} and \mathbf{W}' with eigenvalues β and β' . That is, modes are orthogonal *if their eigenvalues are not complex conjugates*. Moreover, since $i\hat{D}$ is *purely real*, the eigenvalues must come in complex-conjugate pairs. This very useful, because it means if we want a field “parallel” to some eigenfield \mathbf{W} and orthogonal to all the other eigenfields, we just use the eigenfield with the conjugate eigenvalue to \mathbf{W} . And since D is real, that is just \mathbf{W}^* ! So, in short, we have:

$$(\mathbf{W}^*, \mathbf{W}') = 0$$

for distinct eigenvectors \mathbf{W} and \mathbf{W}' : the eigenvectors are orthogonal under the *unconjugated “inner product.”*

Why have we gone through all this analysis of what seems like a rather odd problem? Because this is a simpler version of something that turns out to be extremely useful in more complicated wave equations. In particular, the z -propagation version of the time-harmonic Maxwell equations plays a central role in understanding waveguides and “coupled-wave theory” in electromagnetism [16].

⁷Actually, we only need it to be periodic in z , in which case we can look for Bloch modes.

⁸It is possible to have *standing-wave* modes with real β and $(\mathbf{W}, \mathbf{W}) = 0$, but these mainly occur at $\beta = 0$ (where symmetry causes the flux to be zero).

References

- [1] I. Gohberg, S. Goldberg, and M. A. Kaashoek, *Basic Classes of Linear Operators*. Basel: Birkhäuser, 2000.
- [2] C. Cohen-Tannoudji, B. Din, and F. Laloë, *Quantum Mechanics*. Paris: Hermann, 1977.
- [3] M. Tinkham, *Group Theory and Quantum Mechanics*. New York: Dover, 2003.
- [4] T. Inui, Y. Tanabe, and Y. Onodera, *Group Theory and Its Applications in Physics*. Heidelberg: Springer, 1996.
- [5] Z. Bai, J. Demmel, J. Dongarra, A. Ruhe, and H. Van Der Vorst, eds., *Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide*. Philadelphia: SIAM, 2000.
- [6] R. J. Potton, “Reciprocity in optics,” *Reports Prog. Phys.*, vol. 67, pp. 717–754, 2004.
- [7] J. D. Jackson, *Classical Electrodynamics*. New York: Wiley, third ed., 1998.
- [8] J. D. Joannopoulos, R. D. Meade, and J. N. Winn, *Photonic Crystals: Molding the Flow of Light*. Princeton Univ. Press, 1995.
- [9] L. Landau, E. M. Lifshitz, and L. P. Pitaevskii, *Electrodynamics of Continuous Media*. Oxford: Butterworth-Heinemann, 2nd ed., 1984.
- [10] J. J. Sakurai, *Modern Quantum Mechanics*. Reading, MA: Addison-Wesley, revised ed., 1994.
- [11] C. Kittel, *Introduction to Solid State Physics*. New York: Wiley, 1996.
- [12] N. W. Ashcroft and N. D. Mermin, *Solid State Physics*. Philadelphia: Holt Saunders, 1976.
- [13] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity*. London: Pergamon, 1959.
- [14] W. S. Slaughter, *The Linearized Theory of Elasticity*. Boston: Birkhäuser, 2002.
- [15] M. M. Sigalas and E. N. Economou, “Elastic and acoustic wave band structure,” *J. Sound and Vibration*, vol. 158, no. 2, pp. 377–382, 1992.
- [16] S. G. Johnson, P. Bienstman, M. Skorobogatiy, M. Ibanescu, E. Lidorikis, and J. D. Joannopoulos, “Adiabatic theorem and continuous coupled-mode theory for efficient taper transitions in photonic crystals,” *Phys. Rev. E*, vol. 66, p. 066608, 2002.