Band structure of absorptive photonic crystals

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Abstract. The band structure of absorptive dielectric photonic crystals is investigated. Provided the frequency-dependent electric permeability $\varepsilon(x, \omega)$ satisfies certain analyticity requirements as a function of frequency, we show that no bandgaps exist in frequency regions where absorption takes place, i.e. where $\varepsilon(x, \omega)$ has a non-zero imaginary part. In this case real eigenvalues of the Helmholtz operator in the Bloch-decomposed formalism are absent. Using a suitable analytic continuation procedure, we find that the former change into resonances, i.e. complex numbers depending on k, the wavevector from the first Brillouin zone, thus leading to complex bands in the lower half plane. This is confirmed numerically for a simple, one-dimensional example.

1. Introduction

1.1. Background

Photonic crystals [1] are electromagnetic structures possessing some form of spatial periodicity. Among these the probably best known ones are conservative (non-absorbing) dielectrics with a spatially periodic electric permeability $\varepsilon(x)$. Then, like the spectrum of a Schrödinger operator with a periodic potential, the spectrum of the associated Helmholtz operator has a band structure. Bandgaps may exist and at present there is much activity concerning their calculation and the actual fabrication of bandgap materials. There are a number of reasons which make such systems interesting. We mention the possibility of inhibiting radiative decay of atoms by single photon emission. Indeed, if an atom is embedded in a bandgap dielectric and an atomic transition frequency falls in a gap, then there are no field modes available to carry away the energy. Second, if the bandgap crystal is randomized (for instance by creating impurities) spectrum can develop in the gap and here Anderson localization can occur [2]. Technological applications are foreseen in the areas of optical switches and limiters, superprisms and collimators, new types of displays, solid state lasers, templates for waveguides, solar cells and, eventually, optical chips, whereas enhanced absorption can be very useful in solar energy collectors.

In general $\varepsilon = \varepsilon(x, \omega)$ is a frequency-dependent, complex quantity and absorption can take place. We distinguish three cases. The first is that of conservative systems, where ε does not depend on ω and hence the electromagnetic energy is conserved. Second, transparent or

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dispersive systems are characterized by a frequency dependent but real ε and, finally, absorptive systems are those with a frequency dependent, non-real ε. Obviously ε can be constant, dispersive or absorptive in specific frequency intervals. To those we refer as conservative, dispersive and absorptive intervals. We note that causality implies that a material can never be fully dispersive.

A typical photonic crystal consists of a background medium (permeability ε_b) with non-overlapping spheres or other objects (permeability ε_s) on lattice sites. Promising ways to actually fabricate such systems for optical frequencies can be found using colloid [3] and holographic techniques [4]. Band structure calculations for conservative systems [5] have revealed that an appreciable contrast $\varepsilon_s/\varepsilon_b$ is required for gaps to open and that the situation is most favourable if $\varepsilon_b \gg \varepsilon_s$. This more or less excludes their occurrence in the optical region for ordinary dielectrics. However, it was recently found by one of us [6], that the situation improves dramatically if spheres made up from certain metals or semiconductors are used. For the latter it is known, from both experiment and theory, that Re ε, the real part of ε, can become zero and even quite negative in an appreciable part of the optical region, while absorption remains moderate. Calculations in which absorption was neglected, i.e. Im ε was set to zero, showed that significant optical bandgaps become possible. Earlier work where absorption is included [7] is rather restrictive (one- and two-dimensional systems, small absorption, small filling fraction). See also [8, 9] for recent accounts. In general, if there is appreciable absorption, it is not evident what will happen, in particular whether bandgaps will remain. In the present work we investigate this situation and obtain a negative result: *there are no bandgaps in absorptive frequency ranges*. At first sight this may look surprising but it can be understood by once again considering an excited embedded atom. In the conservative case it can decay provided there are field modes available to propagate away the excitation energy. But in the absorptive case the energy can be transferred to the medium locally, i.e., propagating field modes are not required. However, it is not obvious that this mechanism works, since primarily the atom is coupled to the electromagnetic field and not directly to the medium.

1.2. Bandgaps and analytic continuation

Let us now specify what we mean with a bandgap in the absorptive case. Although it is simply a gap in the spectrum of the Helmholtz operator for a conservative dielectric, this definition needs revision if absorption is present. Thus we consider Maxwell's equations for a linear dielectric,

$$\partial_t \boldsymbol{D}(\boldsymbol{x}, t) = \partial_{\boldsymbol{x}} \times \boldsymbol{B}(\boldsymbol{x}, t) \qquad \partial_t \boldsymbol{B}(\boldsymbol{x}, t) = -\partial_{\boldsymbol{x}} \times \boldsymbol{E}(\boldsymbol{x}, t) \qquad \partial_{\boldsymbol{x}} \cdot \boldsymbol{B}(\boldsymbol{x}, t_0) = 0 \quad (1.1)$$

with

$$\boldsymbol{D}(\boldsymbol{x}, t) = \begin{cases} \varepsilon(\boldsymbol{x})\boldsymbol{E}(\boldsymbol{x}, t) & \text{conservative systems} \\ \boldsymbol{E}(\boldsymbol{x}, t) + \displaystyle\int_{t_0}^{t} \mathrm{d}s \, \chi(\boldsymbol{x}, t - s)\boldsymbol{E}(\boldsymbol{x}, s) & \text{absorptive and dispersive systems} \end{cases}$$

$$(1.2)$$

where $t \geqslant t_0$ with t_0 some initial time and $\chi(\boldsymbol{x}, t)$ is the electric susceptibility. Causality requires that only its values for $t \geqslant 0$ enter in (1.2). Introducing Laplace transforms according to

$$\hat{f}(z) = \begin{cases} \displaystyle\int_{0}^{\infty} \mathrm{d}t \, \exp[\mathrm{i}zt] f(t) & \text{Im } z > 0 \\ \displaystyle\int_{-\infty}^{0} \mathrm{d}t \, \exp[\mathrm{i}zt] f(t) & \text{Im } z < 0 \end{cases} \qquad (1.3)$$

and setting $t_0 = 0$, it follows from Maxwell's equations that

$$[z^2 \varepsilon(\boldsymbol{x}, z) - \mathsf{H}_0]\hat{\boldsymbol{E}}(\boldsymbol{x}, z) = \mathrm{i}z\boldsymbol{E}(\boldsymbol{x}, 0) - \partial_{\boldsymbol{x}} \times \boldsymbol{B}(\boldsymbol{x}, 0) \qquad \mathrm{Im}\, z > 0. \quad (1.4)$$

Here

$$\varepsilon(\boldsymbol{x}, z) = 1 + \hat{\chi}(\boldsymbol{x}, z) \qquad \mathrm{Im}\, z > 0 \qquad \varepsilon_{\mathrm{stat}}(\boldsymbol{x}) = 1 + \chi_{\mathrm{stat}}(\boldsymbol{x})$$

$$\chi_{\mathrm{stat}}(\boldsymbol{x}) = 1 + \int_0^\infty \mathrm{d}t\, \chi(\boldsymbol{x}, t) \qquad\qquad\qquad\qquad\qquad\qquad (1.5)$$

and

$$\mathsf{H}_0 = -\partial_x^2 \mathsf{I} + \partial_{\boldsymbol{x}}\partial_{\boldsymbol{x}} = \boldsymbol{p}^2 \mathsf{I} - \boldsymbol{pp} \qquad \boldsymbol{p} = -\mathrm{i}\partial_{\boldsymbol{x}} \qquad (1.6)$$

where I is the unit 3×3-matrix. In the following we refer to

$$z^2 \varepsilon(\boldsymbol{x}, z) - \mathsf{H}_0 \qquad (1.7)$$

as the Helmholtz operator and, if it exists, write

$$\mathsf{R}_e(z) = [z^2 \varepsilon(\boldsymbol{x}, z) - \mathsf{H}_0]^{-1} \qquad (1.8)$$

for its inverse (this operator was introduced earlier in [10] as $\mathsf{R}_e(z^2)$ but that notation is ambiguous since $\varepsilon(\boldsymbol{x}, z)$ is then not uniquely defined). Then

$$\hat{\boldsymbol{E}}(\boldsymbol{x}, z) = \mathsf{R}_e(z)\{\mathrm{i}z\boldsymbol{E}(\boldsymbol{x}, 0) - \partial_{\boldsymbol{x}} \times \boldsymbol{E}(\boldsymbol{x}, 0)\} \qquad \mathrm{Im}\, z > 0. \quad (1.9)$$

We note in passing that $\mathsf{R}_e(z)$ plays a role in expressions for single photon decay of embedded atoms in dielectrics. To leading order the decay rate for an atom situated in $\boldsymbol{x}$ turns out to be proportional to [10, 11]

$$\mathsf{N}_f(\boldsymbol{x}, \omega) = (2\pi)^{-1}\mathrm{Im}\, \langle \boldsymbol{x}|\mathsf{R}_e(\omega + \mathrm{i}0)|\boldsymbol{x}\rangle \qquad (1.10)$$

which is the local density of states in the conservative situation. Observing that in that case bandgaps are related to the absence of propagating field modes in a certain frequency interval, we are led to the following general definition.

Definition. *We shall say that $\Delta_+ = (\omega_1, \omega_2)$, $0 < \omega_1 < \omega_2$, is a bandgap, if for all allowed $\boldsymbol{E}(\boldsymbol{x}, 0)$, $\boldsymbol{B}(\boldsymbol{x}, 0)$ the fields $\boldsymbol{E}(\boldsymbol{x}, t)$ and $\boldsymbol{B}(\boldsymbol{x}, t)$ have vanishing Fourier components $\tilde{\boldsymbol{E}}(\boldsymbol{x}, \omega)$ and $\tilde{\boldsymbol{B}}(\boldsymbol{x}, \omega)$ for $\omega \in \Delta_+$. The fields being real, $\Delta_- = (-\omega_2, -\omega_1)$ is also a gap, so we are dealing with a bandgap pair $\Delta_\pm$.*

Here and in the following Fourier transforms are defined according to

$$\tilde{f}(\omega) = (2\pi)^{-1}\int_{-\infty}^{+\infty} \mathrm{d}t\, \exp[\mathrm{i}\omega t]f(t) \qquad \omega \in \mathbb{R}. \qquad (1.11)$$

Remark. Note that this definition requires the values of the fields for all $t \in \mathbb{R}$, whereas in (1.1) and (1.2) $t \geqslant t_0$, thus requiring $t_0 = -\infty$. However, as will become clear in section 2, the backward time evolution starting from some finite t_0 is still well defined and hence the Fourier transforms make sense in this case as well.

In the conservative case the above definition is equivalent to the absence of solutions φ_ω of the Helmholtz equation

$$[\omega^2 \varepsilon(\boldsymbol{x}) - \mathsf{H}_0] \cdot \varphi_\omega = 0 \qquad (1.12)$$

for ω in such intervals. There the actual determination of bandgaps follows the same pattern as in solid state physics [5]: the periodicity of $\varepsilon(\boldsymbol{x})$ allows a Bloch decomposition and then (1.12) is solved numerically for $\boldsymbol{x}$ in the unit cell $\mathcal{C}$ with boundary conditions involving $\boldsymbol{k} \in \mathcal{B}$, the first Brillouin zone (for precise definitions, see section 4). If there are no solutions for $\omega \in \Delta$ for

any $k \in \mathcal{B}$, then Δ is a bandgap. This still works for dispersive intervals where $\varepsilon = \varepsilon(x, \omega)$ is real. In the absorptive case one is tempted to consider the Bloch-decomposed version of (1.12) with $\varepsilon(x)$ replaced by the frequency-dependent, complex

$$\varepsilon(x, \omega) = 1 + \hat{\chi}(x, \omega + i0) \qquad \hat{\chi}(x, \omega + i0) = \int_0^\infty dt \, \exp[i\omega t] \chi(x, t) \qquad (1.13)$$

i.e. of

$$[\omega^2 \varepsilon(x, \omega) - H_0(k)] \cdot \varphi_\omega(x, k) = 0. \qquad (1.14)$$

Below we show that this equation has no solutions if $\operatorname{Im} \varepsilon(x, \omega) \neq 0$, provided some analyticity conditions for $\omega \to z \in \mathbb{C}$ are met. The absence of solutions is readily verified for the spatially homogeneous case, $\varepsilon(x, \omega) = \varepsilon(\omega)$, independent of x, by taking the inner product of (1.14) with φ_ω. For ω with $\operatorname{Im} \varepsilon(\omega) \neq 0$ its imaginary part vanishes, implying that $\varphi_\omega = 0$. Of course, this does not mean that the time evolution problem has no solution. In fact we here have the explicit equations

$$E(x, t) = \operatorname{Re} \int d\omega \int dy \frac{1}{8\pi^2 |x - y|}$$
$$\times \exp\left[-i\omega t + i\sqrt{\omega^2 \varepsilon(\omega)} |x - y|\right] \{i\omega E(y, 0) - (\partial_x \times B)(y, 0)\} \qquad (1.15)$$

$$\tilde{E}(x, \omega) = \operatorname{Re} \int dy \frac{1}{8\pi^2 |x - y|} \exp\left[i\sqrt{\omega^2 \varepsilon(\omega)} |x - y|\right] \{i\omega E(y, 0) - (\partial_x \times B)(y, 0)\}$$

where the only effect of absorption is the damping term $-\operatorname{Im} \sqrt{\omega^2 \varepsilon(\omega)} |x - y|$ in the exponential.

One might think that (1.14) has solutions for non-real ω. This is not the case for $\operatorname{Im} \omega > 0$, whereas $\hat{\chi}(x, \omega)$ must posses an analytic continuation for $\operatorname{Im} \omega < 0$ in order to find solutions with $\operatorname{Im} \omega < 0$. As discussed in sections 6 and 7 it is then possible to find complex eigenvalues, but not in direct connection with (1.14). Finally, complex vectors k in a Bloch decomposition come to mind. But if we reconstruct $\varphi_\omega(x)$ from such $\varphi_\omega(x, k)$, we find that it blows up for certain x-directions, which is undesirable. Indeed, in (1.15) the kernel remains well behaved and an expansion in terms of such unbounded $\varphi_\omega(x)$ becomes problematic.

However, whatever the status is for the solutions of (1.14), the bandgap problem is well defined as we shall now discuss. In section 2 it is shown that ($z = \omega + i\delta, \delta > 0$)

$$\tilde{E}(\omega) = \lim_{\delta \downarrow 0} (2\pi)^{-1} [\{R_e(z) - R_e(z)^*\} \{i\omega E(0) - \partial_x \times B(0)\} - \{R_e(z) + R_e(z)^*\} \delta E(0)]$$

$$(1.16)$$

so that, provided

$$R_e(\omega) = \lim_{\delta \downarrow 0} R_e(\omega + i\delta) \qquad \omega \in \mathbb{R} \qquad (1.17)$$

exists,

$$\tilde{E}(\omega) = \lim_{\delta \downarrow 0} (2\pi)^{-1} \{R_e(z) - R_e(z)^*\} \{i\omega E(0) - \partial_x \times B(0)\}$$
$$= -i\omega^2 \pi^{-1} R_e(\omega)^* \operatorname{Im} \varepsilon(x, \omega) R_e(\omega) \{i\omega E(0) - \partial_x \times B(0)\}. \qquad (1.18)$$

Thus we expect that $\tilde{E}(\omega) \neq 0$ for $\omega \in \Delta$, where Δ is an interval on which $\operatorname{Im} \varepsilon(x, \omega)$ is non-zero, i.e. Δ cannot be a bandgap. In actuality the situation is somewhat more subtle, as discussed in section 4. On the other hand, if $\varepsilon(x, \omega)$ is dispersive on the open interval Δ', i.e. $\operatorname{Im} \varepsilon(x, \omega)$ vanishes for $\omega \in \Delta'$, then $R_e(\omega)$ may not exist for $\omega \in \Delta'$, in which case (1.18) does not apply and Δ' may contain bandgaps. It will be clear that the actual situation depends critically on $R_e(z)$ and its limiting properties as z approaches the real axis. Our analysis will

make use of the circumstance that $\mathsf{R}_e(z)$ can be represented as a projection of the resolvent of a selfadjoint operator $\mathsf{H}_e \geqslant 0$ in a suitable Hilbert space,

$$\mathsf{R}_e(z) = P_1[z^2 - \mathsf{H}_e]^{-1}P_1 \qquad \operatorname{Im} z > 0 \qquad (1.19)$$

where P_1 is a projector. This procedure was used earlier in [10] and is briefly recapitulated in section 2. In section 3 we discuss H_e in some detail as a preparation for the Bloch decomposition that will be made in section 4. The latter is used in sections 5–7, where we make some analytic continuation assumptions about $\hat{\chi}(z)$. In section 5 we give a precise statement about the absence of bandgaps in the absorptive case and also show that in that situation (1.14) has no solutions for ω with $\operatorname{Im} \varepsilon(x, \omega) > 0$. Instead it is possible to continue $\mathsf{R}_e(z, \boldsymbol{k})$, the Bloch-decomposed version of $\mathsf{R}_e(z)$, analytically across the real axis and obtain the representation

$$\mathsf{R}_e(z, \boldsymbol{k}) = z^{-1}\mathsf{A}_0 + \sum_r [z - \lambda_r(\boldsymbol{k})]^{-1}\mathsf{A}_r(\boldsymbol{k}) + \mathsf{R}'_e(z, \boldsymbol{k}) \qquad \operatorname{Im} z > 0. \quad (1.20)$$

Here $\operatorname{Im} \lambda_r(\boldsymbol{k}) \leqslant 0$ and, for $r \neq 0$, the $\mathsf{A}_r(\boldsymbol{k})$ are finite-dimensional operators, whereas the background term $\mathsf{R}'_e(z, \boldsymbol{k})$ is analytic. Thus the sets $\{\lambda_r(\boldsymbol{k})|\boldsymbol{k} \in \mathcal{B}\}$, where $\mathcal{B}$ is the first Brillouin zone, form bands in the lower half plane. An improved result is obtained in section 7, where $\mathsf{H}_e(\boldsymbol{k})$, the Bloch-decomposed version of H_e, is studied. After a complex dilatation transformation, $\mathsf{H}_e(\boldsymbol{k}) \rightarrow \mathsf{H}_e(\boldsymbol{k}, \zeta)$, the resolvent $[z^2 - \mathsf{H}_e(\boldsymbol{k}, \zeta)]^{-1}$ is continued across the real axis and resonances (complex eigenvalues of $\mathsf{H}_e(\boldsymbol{k}, \zeta)$ in the lower half plane) $\lambda_r(\boldsymbol{k})$ can emerge. They can be interpreted, at least for weak absorption, as originating from the poles of $[z^2 - \mathsf{H}_0(\boldsymbol{k})]^{-1}$, i.e. the eigenvalues of the 'free' Bloch-decomposed $\mathsf{H}_0(\boldsymbol{k})$. The complex-dilated version of (1.17) then relates the $\mathsf{A}_r(\boldsymbol{k})$s to the eigenvectors of $\mathsf{H}_e(\boldsymbol{k}, \zeta)$. Note that in the conservative case no analytic continuation is required, the background term $\mathsf{R}'_e(z, \boldsymbol{k})$ is absent, and the $\lambda_r(\boldsymbol{k})$ are real, giving rise to real bands, whereas the $\mathsf{A}_r(\boldsymbol{k})$ are mutually orthogonal projectors. Our findings were confirmed by a numerical study of a simple one-dimensional model.

2. Auxiliary fields and energy conservation

Absorption is a phenomenon where energy is transferred from a subsystem A to another B in a one-way fashion. The overall energy may be conserved but usually system B is eliminated from the formalism and we end up with a so-called open system. Given its behaviour one might try to reconstruct the full system A + B but in many cases this is no longer possible in a unique way; too much information is lost. A typical example is the damped harmonic operator. The situation is more favourable in the absorptive Maxwell case and other situations where absorption is brought in through a convolutive term in the time evolution. We note that even for a conservative dielectric it is not the purely electromagnetic quantity

$$\mathfrak{E}_{\text{em}} = \tfrac{1}{2} \int \mathrm{d}x \, \{E(x, t)^2 + B(x, t)^2\} \qquad (2.1)$$

that is conserved, but rather

$$\mathfrak{E} = \tfrac{1}{2} \int \mathrm{d}x \, \{E(x, t) \cdot D(x, t) + B(x, t)^2\} \qquad (2.2)$$

which contains the polarization $P(x, t)$ through

$$D(x, t) = E(x, t) + P(x, t). \qquad (2.3)$$

As one of us (Tip [10]) recently showed, there also exists a conserved quantity in the absorptive case. It no longer involves the polarization directly but rather two new fields that depend on x, t and a new variable $\lambda \in \mathbb{R}$. We start our discussion by making a few assumptions, which are

usually justified in actual physical systems. Later on some further assumptions will be made (below $\mathbb{R}^+$ and $\mathbb{R}^-$ are the open positive and negative half axis, $\overline{\mathbb{R}}^+ = [0, \infty)$, whereas $\mathbb{C}^+$ and $\mathbb{C}^-$ are the open upper and lower complex half planes).

A_1: $\chi(\boldsymbol{x}, t)$, $\mathbb{R}^3 \times \mathbb{R}^+ \to \mathbb{R}$ is a measurable function, continuous in $t \geqslant 0$ with $\chi(\boldsymbol{x}, 0) = 0$ differentiable in $t > 0$, right differentiable in $t = 0$, and absolutely integrable:

$$\int_0^\infty \mathrm{d}t \, |\chi(\boldsymbol{x}, t)| \leqslant c_1 < \infty.$$

Consequently $\hat{\chi}(\boldsymbol{x}, z)$ exists for $\mathrm{Im}\, z > 0$ and has limits for $\mathrm{Im}\, z \downarrow 0$. This also guarantees the existence of $\varepsilon_{\mathrm{stat}}(\boldsymbol{x})$.

A_2: $\chi'(\boldsymbol{x}, t) \equiv \partial_t \chi(\boldsymbol{x}, t)$ has a representation (λ-integrals are over $\mathbb{R}$ unless stated differently)

$$\chi'(\boldsymbol{x}, t) = \int \mathrm{d}\lambda \, \nu(\boldsymbol{x}, \lambda) \cos \lambda t \qquad t \geqslant 0$$

with $\nu(\boldsymbol{x}, \lambda)$, continuous in λ, satisfying

$$\nu(\boldsymbol{x}, \lambda) = \nu(\boldsymbol{x}, -\lambda) \geqslant 0 \qquad \int \mathrm{d}\lambda \, (1 + |\lambda|)\nu(\boldsymbol{x}, \lambda) \leqslant c_2 < \infty.$$

It follows that $\chi'(\boldsymbol{x}, t)$ is continuous in t and tends to zero as $|t| \to \infty$ and also that $\chi(\boldsymbol{x}, t)$ is twice differentiable for $t > 0$. For later reference we give a list of properties based upon the above assumptions, valid for $t \geqslant 0$ and $\mathrm{Im}\, z > 0$ where applicable:

$$\chi(\boldsymbol{x}, t) = \int \mathrm{d}\lambda \, \lambda^{-1} \nu(\boldsymbol{x}, \lambda) \sin \lambda t \qquad \chi(\boldsymbol{x}, 0) = 0$$

$$\chi'(\boldsymbol{x}, t) = \int \mathrm{d}\lambda \, \nu(\boldsymbol{x}, \lambda) \cos \lambda t \qquad \chi'(\boldsymbol{x}, 0) = \int \mathrm{d}\lambda \, \nu(\boldsymbol{x}, \lambda)$$

$$\hat{\chi}(\boldsymbol{x}, z) = z^{-1} \int \mathrm{d}\lambda \, [\lambda - z]^{-1} \nu(\boldsymbol{x}, \lambda) = \int \mathrm{d}\lambda \, [\lambda^2 - z^2]^{-1} \nu(\boldsymbol{x}, \lambda)$$

$$\hat{\chi}(\boldsymbol{x}, 0) = \int \mathrm{d}\lambda \, \lambda^{-2} \nu(\boldsymbol{x}, \lambda)$$

(2.4)

$$\varepsilon(\boldsymbol{x}, \omega) = 1 + \hat{\chi}(\boldsymbol{x}, \omega + \mathrm{i}0) \qquad \mathrm{Im}\, \varepsilon(\boldsymbol{x}, \omega) = \mathrm{Im}\, \hat{\chi}(\boldsymbol{x}, \omega + \mathrm{i}0) = \pi \nu(\boldsymbol{x}, \omega)/\omega$$

$$\nu(\boldsymbol{x}, \lambda) = \pi^{-1} \int_0^\infty \mathrm{d}t \cos \lambda t \, \chi'(\boldsymbol{x}, t) \qquad \nu(\boldsymbol{x}, 0) = 0.$$

With $\boldsymbol{F}_1(\boldsymbol{x}, t) = \boldsymbol{E}(\boldsymbol{x}, t)$, $\boldsymbol{F}_3(\boldsymbol{x}, t) = \boldsymbol{B}(\boldsymbol{x}, t)$ and $\boldsymbol{F}_2(\boldsymbol{x}, t, \lambda)$ and $\boldsymbol{F}_4(\boldsymbol{x}, t, \lambda)$ the two new fields, the set

$$\partial_t \boldsymbol{F}_1(\boldsymbol{x}, t) = \partial_{\boldsymbol{x}} \times \boldsymbol{F}_3(\boldsymbol{x}, t) + \int \mathrm{d}\lambda \, \sigma(\boldsymbol{x}, \lambda) \boldsymbol{F}_4(\boldsymbol{x}, t, \lambda)$$

$$\partial_t \boldsymbol{F}_2(\boldsymbol{x}, t, \lambda) = \lambda \boldsymbol{F}_4(\boldsymbol{x}, t, \lambda)$$

$$\partial_t \boldsymbol{F}_3(\boldsymbol{x}, t) = -\partial_{\boldsymbol{x}} \times \boldsymbol{F}_1(\boldsymbol{x}, t)$$

$$\partial_t \boldsymbol{F}_4(\boldsymbol{x}, t, \lambda) = -\sigma(\boldsymbol{x}, \lambda) \boldsymbol{F}_1(\boldsymbol{x}, t) - \lambda \boldsymbol{F}_2(\boldsymbol{x}, t, \lambda)$$

(2.5)

where $\sigma(\boldsymbol{x}, \lambda)^2 = \nu(\boldsymbol{x}, \lambda)$, $\sigma(\boldsymbol{x}, \lambda) \geqslant 0$ and $\boldsymbol{F}_2(\boldsymbol{x}, t_0, \lambda) = \boldsymbol{F}_4(\boldsymbol{x}, t_0, \lambda) = 0$, is equivalent with the original set of absorptive Maxwell's equations. This is readily checked by expressing the new fields in terms of the electromagnetic ones, using the second and last of these equations, giving

$$\boldsymbol{F}_2(\boldsymbol{x}, t, \lambda) = -\sigma(\boldsymbol{x}, \lambda) \int_{t_0}^t \mathrm{d}s \sin \lambda(t - s) \boldsymbol{E}(\boldsymbol{x}, s)$$

$$\boldsymbol{F}_4(\boldsymbol{x}, t, \lambda) = -\sigma(\boldsymbol{x}, \lambda) \int_{t_0}^t \mathrm{d}s \cos \lambda(t - s) \boldsymbol{E}(\boldsymbol{x}, s)$$

and substitution into the first. Moreover the quantity

$$\mathfrak{E} = \tfrac{1}{2} \int \mathrm{d}\boldsymbol{x} \, \{ \boldsymbol{F}_1(\boldsymbol{x}, t)^2 + \boldsymbol{F}_3(\boldsymbol{x}, t)^2 \}$$

$$+ \tfrac{1}{2} \int \mathrm{d}\boldsymbol{x} \int \mathrm{d}\lambda \, \{ \boldsymbol{F}_2(\boldsymbol{x}, t, \lambda)^2 + \boldsymbol{F}_4(\boldsymbol{x}, t, \lambda)^2 \} = \mathfrak{E}_{\mathrm{em}} + \mathfrak{E}_{aux} \tag{2.6}$$

which reduces to the electromagnetic energy in the vacuum case ($\chi(\boldsymbol{x}, t) \equiv 0$), is conserved in time. Since now

$$\boldsymbol{P}(\boldsymbol{x}, t) = - \int \mathrm{d}\lambda \, \lambda^{-1} \sigma(\boldsymbol{x}, \lambda) \boldsymbol{F}_2(\boldsymbol{x}, t, \lambda) \tag{2.7}$$

this expression essentially differs from (2.2) above. In [10] these results were used as a starting point to construct a Hilbert space set-up followed by the introduction of a canonical formalism and its quantization. Here we only need the first part. Thus the set (2.5) above is interpreted as a time evolution equation,

$$\partial_t \boldsymbol{F}(t) = -\mathrm{i}\mathsf{K}\boldsymbol{F}(t) \qquad t > 0 \tag{2.8}$$

in the Hilbert space $\mathcal{K} = \oplus_{j=1}^4 \mathcal{H}_j$, $\mathcal{H}_1 = \mathcal{H}_3 = L^2(\mathbb{R}^3, \mathrm{d}\boldsymbol{x}; \mathbb{C}^3)$, $\mathcal{H}_2 = \mathcal{H}_4 = L^2(\mathcal{A}, \mathrm{d}\boldsymbol{x}; \mathbb{C}^3) \otimes L^2(\mathbb{R}, \mathrm{d}\lambda)$. Thus we are dealing with four square integrable, three-dimensional, complex vector fields. The $\boldsymbol{x}$-integration for the auxiliary fields is restricted to $\mathcal{A}$, the closed complement in $\mathbb{R}^3$ of the set $\{\boldsymbol{x} \in \mathbb{R}^3 \,|\, \chi(\boldsymbol{x}, t) = 0, \forall t \in \mathbb{R}^+\}$, i.e. the auxiliary fields only live inside the absorbing material. Alternatively we can set $\mathcal{H}_2 = \mathcal{H}_4 = L^2(\mathbb{R}^3, \mathrm{d}\boldsymbol{x}; \mathbb{C}^3) \otimes L^2(\mathbb{R}, \mathrm{d}\lambda)$, provided we replace $\boldsymbol{F}_{2,4}$ by $\Psi_{\mathcal{A}}(\boldsymbol{x})\lambda \boldsymbol{F}_{2,4}$ in (2.5). Here $\Psi_{\mathcal{C}}$ is the characteristic function for the set $\mathcal{C}$: $\Psi_{\mathcal{C}}(c) = 1$ for $c \in \mathcal{C}$ and zero otherwise.

Proposition 2.1. *Suppose A_1 and A_2 are satisfied. Then K defines a selfadjoint operator in $\mathcal{K}$.*

Proof. We split K according to

$$\mathsf{K} = \mathsf{K}_0 + \mathsf{K}_1 \tag{2.9}$$

where

$$\mathsf{K}_0 = \begin{pmatrix} 0 & 0 & \boldsymbol{\epsilon} \cdot \boldsymbol{p} & 0 \\ 0 & 0 & 0 & \mathrm{i}\lambda \\ -\boldsymbol{\epsilon} \cdot \boldsymbol{p} & 0 & 0 & 0 \\ 0 & -\mathrm{i}\lambda & 0 & 0 \end{pmatrix} \tag{2.10}$$

with $\boldsymbol{\epsilon} = \{\epsilon_{ijk}\}$ the Levi-Civita pseudo-tensor, antisymmetric under an interchange of each pair of indices and $\epsilon_{123} = 1$, and

$$\mathsf{K}_1 = \begin{pmatrix} 0 & 0 & 0 & \mathrm{i} \int \mathrm{d}\lambda \, \sigma(\boldsymbol{x}, \lambda), \ldots \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\mathrm{i}\sigma(\boldsymbol{x}, \lambda) & 0 & 0 & 0 \end{pmatrix}. \tag{2.11}$$

K_0 is selfadjoint since it becomes a Hermitean matrix-valued multiplication operator if $\mathcal{H}_1$ and $\mathcal{H}_3$ are mapped onto their momentum space versions $L^2(\mathbb{R}^3, \mathrm{d}\boldsymbol{p}; \mathbb{C}^3)$. In addition, K_1 is symmetric on the domain $\mathcal{D}(\mathsf{K}_0)$ of K_0. It is also bounded since, for $\boldsymbol{f} \in \mathcal{K}$,

$$\|\mathsf{K}_1 \boldsymbol{f}\|^2 = \int \mathrm{d}\boldsymbol{x} \left| \int \mathrm{d}\lambda \, \sigma(\boldsymbol{x}, \lambda) \boldsymbol{f}_4(\boldsymbol{x}, \lambda) \right|^2 + \int \mathrm{d}\boldsymbol{x} \, \mathrm{d}\lambda \, \sigma(\boldsymbol{x}, \lambda)^2 |\boldsymbol{f}_1(\boldsymbol{x})|^2 \leqslant c_1 \|\boldsymbol{f}\|^2.$$

Thus K is selfadjoint with the domain $\mathcal{D}(\mathsf{K}_0)$. $\qquad \square$

Corollary 2.2. *Equation (2.8) has the solution*

$$\boldsymbol{F}(t) = \exp[-iKt]\boldsymbol{F}(0) \qquad t > t_0 \tag{2.12}$$

which extends to a unitary time evolution for all $t \in \mathbb{R}$ if t_0 is finite.

Next we note that

$$\mathsf{K}^2 = \begin{pmatrix} \mathsf{H}_e & 0 \\ 0 & \mathsf{H}_m \end{pmatrix} \tag{2.13}$$

where

$$\mathsf{H}_e = \begin{pmatrix} \mathsf{H}_0 + \chi'(\boldsymbol{x}, 0) & \int d\lambda\, \lambda\sigma(\boldsymbol{x}, \lambda), \dots \\ \lambda\sigma(\boldsymbol{x}, \lambda) & \lambda^2 \end{pmatrix}$$
$$= \begin{pmatrix} \mathsf{H}_0 + \int d\lambda\, \sigma(\boldsymbol{x}, \lambda)^2 & \int d\lambda\, \lambda\sigma(\boldsymbol{x}, \lambda), \dots \\ \lambda\sigma(\boldsymbol{x}, \lambda) & \lambda^2 \end{pmatrix} \tag{2.14}$$

acts in $\mathcal{H}_e = \mathcal{H}_1 \oplus \mathcal{H}_2$ and similar for H_m in $\mathcal{H}_3 \oplus \mathcal{H}_4$ (for further details, see [10]). Now $\boldsymbol{F}(t) = \exp[-iKt]\boldsymbol{F}(0)$ is a bounded, continuous, $\mathcal{K}$-valued function of t, so

$$\boldsymbol{F}_\delta(t) = \exp[-\delta|t|]\boldsymbol{F}(t) \qquad \delta > 0 \tag{2.15}$$

is a square integrable function of t and has the Fourier transform (an element of $L^1(\mathbb{R}, d\omega; \mathcal{H}_e) \cap L^2(\mathbb{R}, d\omega; \mathcal{H}_e)$)

$$\tilde{\boldsymbol{F}}_\delta(\omega) = (2\pi)^{-1} \int_{-\infty}^{+\infty} dt\, \exp[i\omega t]\boldsymbol{F}_\delta(t) = i(2\pi)^{-1}\{[z - \mathsf{K}]^{-1} - [\bar{z} - \mathsf{K}]^{-1}\}\boldsymbol{F}(0)$$
$$= i(2\pi)^{-1}\{[z^2 - \mathsf{K}^2]^{-1}[z + \mathsf{K}] - [\bar{z}^2 - \mathsf{K}^2]^{-1}[\bar{z} + \mathsf{K}]\}\boldsymbol{F}(0)$$
$$= i(2\pi)^{-1}\{[z^2 - \mathsf{K}^2]^{-1} - [\bar{z}^2 - \mathsf{K}^2]^{-1}\}[\omega + \mathsf{K}]\boldsymbol{F}(0)$$
$$\quad - (2\pi)^{-1}\{[z^2 - \mathsf{K}^2]^{-1} + [\bar{z}^2 - \mathsf{K}^2]^{-1}\}\delta\boldsymbol{F}(0) \tag{2.16}$$

where $z = \omega + i\delta$. Let P_j be the projector upon $\mathcal{H}_j \subset \mathcal{K}$. Then $P_{\text{em}} = P_1 + P_3$ is the projector upon the electromagnetic subspace $\mathcal{H}_1 \oplus \mathcal{H}_3$ and, since the auxiliary fields vanish at $t_0 = 0$, for $P_{\text{em}}\boldsymbol{F}(0) \in \mathcal{D}(\mathsf{K})$,

$$P_{\text{em}}\tilde{\boldsymbol{F}}_\delta(\omega) = i(2\pi)^{-1} P_{\text{em}}\{[z^2 - \mathsf{K}^2]^{-1} - [\bar{z}^2 - \mathsf{K}^2]^{-1}\}[\omega + \mathsf{K}]P_{\text{em}}\boldsymbol{F}(0)$$
$$\quad - (2\pi)^{-1} P_{\text{em}}\{[z^2 - \mathsf{K}^2]^{-1} + [\bar{z}^2 - \mathsf{K}^2]^{-1}\}P_{\text{em}}\delta\boldsymbol{F}(0)$$

and in particular, in view of (2.13), with some abuse of notation,

$$\tilde{\boldsymbol{E}}_\delta(\omega) = i(2\pi)^{-1} P_1\{[z^2 - \mathsf{H}_e]^{-1} - [\bar{z}^2 - \mathsf{H}_e]^{-1}\}P_1\{\omega\boldsymbol{E}(0) + \mathsf{K}_{13}\boldsymbol{B}(0)\}$$
$$\quad - (2\pi)^{-1} P_1\{[z^2 - \mathsf{H}_e]^{-1} + [\bar{z}^2 - \mathsf{H}_e]^{-1}\}P_1\delta\boldsymbol{E}(0) \tag{2.17}$$

and a similar expression for $\tilde{\boldsymbol{B}}_\delta(\omega)$. In order to evaluate (2.17) further, we use the Feshbach formula ([12]). It reads, with P a projector, $Q = 1 - P$ and A an operator,

$$A^{-1} = Q[QAQ]^{-1}Q + \{P - Q[QAQ]^{-1}QAP\}\mathcal{G}\{P - PAQ[QAQ]^{-1}Q\}$$
$$\mathcal{G} = [PAP - PAQ[QAQ]^{-1}QAP]^{-1}P \tag{2.18}$$

provided that the inverses make sense and there are no domain problems in case the operators are unbounded. Applying this to (2.17) with $P = P_1$ and $A = z^2 - \mathsf{H}_e$ we arrive at a relation which is essential in the present set-up, i.e. the connection between $[z^2\varepsilon(\boldsymbol{x}, z) - \mathsf{H}_0]^{-1}$ and the resolvent of a selfadjoint operator (see also [10]):

Proposition 2.3.

$$P_1[z^2 - \mathsf{H}_e]^{-1}P_1 = [z^2\varepsilon(\boldsymbol{x}, z) - \mathsf{H}_0]^{-1}P_1 = \mathsf{R}_e(z)P_1$$
$$\varepsilon(\boldsymbol{x}, z) = 1 + \hat{\chi}(\boldsymbol{x}, z) \qquad \text{Im } z > 0. \tag{2.19}$$

Thus

$$\tilde{E}_\delta(\omega) = (2\pi)^{-1}\{\mathsf{R}_e(z) - \mathsf{R}_e(z)^*\}\{i\omega E(0) - \partial_x \times B(0)\} - (2\pi)^{-1}\{\mathsf{R}_e(z) + \mathsf{R}_e(z)^*\}\delta E(0)$$
$$= -i\pi^{-1}\mathsf{R}_e(z)^*\mathrm{Im}\, z^2\varepsilon(x, z)\mathsf{R}_e(z)\{i\omega E(0) - \partial_x \times B(0)\}$$
$$-(2\pi)^{-1}\{\mathsf{R}_e(z) + \mathsf{R}_e(z)^*\}\delta E(0) \tag{2.20}$$

where we used

$$\mathsf{R}_e(z) - \mathsf{R}_e(z)^* = -2i\mathsf{R}_e(z)^*\{\mathrm{Im}\, z^2\varepsilon(x, z)\}\mathsf{R}_e(z). \tag{2.21}$$

Now suppose that the limit

$$\mathsf{R}_e(\omega) = \lim_{\delta\downarrow 0}\mathsf{R}_e(z) \tag{2.22}$$

exists. Then, recalling that $\mathrm{Im}\,\hat{\chi}(x, \omega + i0) = \frac{\pi}{\omega}\nu(x, \omega), 0 \neq \omega \in \mathbb{R}$, we end up with

$$\tilde{E}(\omega) = \lim_{\delta\downarrow 0}\tilde{E}_\delta(\omega) = -i\omega\mathsf{R}_e(\omega + i0)^*\nu(x, \omega)\mathsf{R}_e(\omega + i0)\{i\omega E(0) - \partial_x \times B(0)\}. \tag{2.23}$$

In a similar way

$$\tilde{B}(\omega) = \lim_{\delta\downarrow 0}\tilde{B}_\delta(\omega) = (2\pi)^{-1}\{\mathsf{R}_m(\omega + i0) - \mathsf{R}_m(\omega + i0)^*\}\{i\omega B(0) + \partial_x \times E(0)\} \tag{2.24}$$

where

$$\mathsf{R}_m(z) = [z^2 + (\epsilon \cdot p) \cdot \varepsilon(x, z)^{-1}(\epsilon \cdot p)]^{-1} = z^{-2}\{1 - (\epsilon \cdot p) \cdot \mathsf{R}_e(z) \cdot (\epsilon \cdot p)\} \tag{2.25}$$

so, for $\omega \neq 0$,

$$\tilde{B}(\omega) = i\omega^{-1}(\epsilon \cdot p) \cdot \mathsf{R}_e(\omega + i0)^*\nu(x, \omega)\mathsf{R}_e(\omega + i0) \cdot (\epsilon \cdot p) \cdot \{i\omega B(0) + \partial_x \times E(0)\}. \tag{2.26}$$

In (2.22) we recognize (1.17). However, in view of proposition 2.3, we now know that $\mathsf{R}_e(z)$ is well defined for any $z \in \mathbb{C}^+ = \{z \in \mathbb{C}|\mathrm{Im}\, z > 0\}$. A further advantage is that $\tilde{E}(\omega)$ is expressed in terms of the resolvent $[z^2 - \mathsf{H}_e]^{-1}$ and all properties of interest are related to the operator H_e in $\mathcal{H}_e$, to which we turn in the next section.

3. The operator H_e

As a preliminary we note that in H_e the operator $\mathsf{H}_0 = p^2\mathsf{I} - pp$ enters. In momentum space, $\tilde{\mathcal{H}}_1 = L^2(\mathbb{R}^3, \mathrm{d}p; \mathbb{C}^3)$, it is a simple matrix multiplication operator. The projector upon its (infinite-dimensional) null space (the longitudinal vectors) is $P^\| = e_p e_p$, where $e_a = a/a$, $a = |a|$, and the complementary projector (onto the transverse vectors) is $P^\perp = \Delta_p = \mathsf{I} - e_p e_p$. Then, for $\zeta \in \rho(\mathsf{H}_0)$, the resolvent set of H_0,

$$[\zeta - \mathsf{H}_0]^{-1} = \zeta^{-1}e_p e_p + [\zeta - p^2]^{-1}\Delta_p. \tag{3.1}$$

Although the selfadjointness of H_e follows from general properties [13], given the structure of K, it is instructive to see how it can be obtained directly. We note that the domain $\mathcal{D}(\mathsf{H}_e^{(0)})$ of

$$\mathsf{H}_e^{(0)} = \begin{pmatrix} \mathsf{H}_0 & 0 \\ 0 & \lambda^2 \end{pmatrix} \tag{3.2}$$

consists of vectors $f = (f_1, f_2)$ with $f_1 \in \mathcal{D}(\mathsf{H}_0) \subset \mathcal{H}_1$ and $f_2 \in \mathcal{D}(\lambda^2) \subset \mathcal{H}_2$. For such f we have

$$(\mathsf{H}_e \cdot f, f) = (\mathsf{H}_0 f_1, f_1)_1 + \int \mathrm{d}x \int \mathrm{d}\lambda\, |\sigma(x, \lambda)f_1(x) + \lambda f_2(x, \lambda)|^2 \geqslant 0. \tag{3.3}$$

It will be clear that V in $\mathsf{H}_e = \mathsf{H}_e^{(0)} + \mathsf{V}$, restricted to the form domain of $\mathsf{H}_e^{(0)}$, is relatively form-bounded with zero bound, so $\mathsf{H}_e^{(0)} + \mathsf{V}$ extends to a selfadjoint operator in $\mathcal{H}_e$. Note that V is in general not operator-bounded relative to $\mathsf{H}_e^{(0)}$, since $\|\mathsf{V}f\|^2$ contains the term $\int \mathrm{d}x \int \mathrm{d}\lambda\, \lambda^2\nu(x, \lambda)|f_1(x)|^2$ and $\int \mathrm{d}\lambda\, \lambda^2\nu(x, \lambda)$ need not be finite. It is, however, if we have:

A_3: $\nu(\boldsymbol{x}, \lambda)$ satisfies

$$\int d\lambda \, \lambda^2 \nu(\boldsymbol{x}, \lambda) = -\partial_t^3 \chi(\boldsymbol{x}, t)|_{t=0} \leqslant c_3 < \infty$$

which is the case for many situations of physical interest, such as exponentially decaying, smooth $\chi(t)$.

We note further that it is easy to read off the elements of the null space of H_e from (3.3). They have to satisfy $\mathsf{H}_0 \boldsymbol{f}_1 = 0$, so $\boldsymbol{f}_1$ is longitudinal, and $\boldsymbol{f}_2(\boldsymbol{x}, \lambda) = -\lambda^{-1} \sigma(\boldsymbol{x}, \lambda) \boldsymbol{f}_1(\boldsymbol{x})$, $\lambda \neq 0$. The corresponding projector is given in the appendix.

Finally we turn to the case where $\chi(\boldsymbol{x}, t)$ is constant over $\boldsymbol{x} \in \mathcal{A}$, i.e.

$$\chi(\boldsymbol{x}, t) = \Psi_\mathcal{A}(\boldsymbol{x}) g(t) \qquad t \geqslant 0 \tag{3.4}$$

where, as before, Ψ is a characteristic function and $\mathcal{A}$ the volume occupied by the absorptive medium. Note that $g(0) = 0$. We now have

$$\nu(\boldsymbol{x}, \lambda) = \Psi_\mathcal{A}(\boldsymbol{x}) n(\lambda) \qquad n(\lambda) = s(\lambda)^2 \qquad s(\lambda) \geqslant 0 \qquad \sigma(\boldsymbol{x}, \lambda) = \Psi_\mathcal{A}(\boldsymbol{x}) s(\lambda)$$

$$\hat{\chi}(\boldsymbol{x}, z) = \Psi_\mathcal{A}(\boldsymbol{x}) \hat{g}(z) \qquad \chi'(\boldsymbol{x}, 0) = \Psi_\mathcal{A}(\boldsymbol{x}) \int d\lambda \, n(\lambda) = \Psi_\mathcal{A}(\boldsymbol{x}) \|n\|_1 = \Psi_\mathcal{A}(\boldsymbol{x}) \|s\|^2.$$

$$\tag{3.5}$$

If the above quantities occur as operators, we can write, noting that $\Psi_\mathcal{A}(\boldsymbol{x})$ defines the projector $P_\mathcal{A}$,

$$\nu(\boldsymbol{x}, \lambda) = P_\mathcal{A}(\boldsymbol{x}) n(\lambda) \qquad n(\lambda) = s(\lambda)^2$$

$$\sigma(\boldsymbol{x}, \lambda) = P_\mathcal{A}(\boldsymbol{x}) s(\lambda) \qquad \chi'(\boldsymbol{x}, 0) = P_\mathcal{A}(\boldsymbol{x}) \int d\lambda \, n(\lambda) = P_\mathcal{A}(\boldsymbol{x}) \|n\|_1$$

$$\hat{\chi}(\boldsymbol{x}, z) = P_\mathcal{A}(\boldsymbol{x}) \hat{g}(z) \qquad \hat{g}(z) = \int d\lambda \, [\lambda^2 - z^2]^{-1} n(\lambda) \tag{3.6}$$

$$\hat{g}(\lambda + \mathrm{i}0) = \int_0^\infty dt \, \exp[\mathrm{i}\lambda t] g(t) \qquad \mathrm{Im}\, \hat{g}(\lambda + \mathrm{i}0) = \frac{\pi}{\lambda} n(\lambda)$$

where $\mathrm{Im}\, z > 0$. H_e can now be written in the suggestive way ($\langle s|\lambda|f \rangle = \int d\lambda \, s(\lambda) f(\lambda)$, etc)

$$\mathsf{H}_e = \begin{pmatrix} \mathsf{H}_0 + P_\mathcal{A} \|n\|_1 & P_\mathcal{A} \langle s|\lambda \\ P_\mathcal{A} \lambda |s\rangle & \lambda^2 \end{pmatrix}. \tag{3.7}$$

In view of the Bloch–Floquet decomposition, to be discussed below, it is convenient to change $\mathcal{H}_2 = L^2(\mathcal{A}, d\boldsymbol{x}; \mathbb{C}^3) \otimes L^2(\mathbb{R}, d\lambda)$ into $\mathcal{H}_2 = L^2(\mathbb{R}^3, d\boldsymbol{x}; \mathbb{C}^3) \otimes L^2(\mathbb{R}, d\lambda)$ and replace H_e by

$$\mathsf{H}_e = \begin{pmatrix} \mathsf{H}_0 + P_\mathcal{A} \|n\|_1 & P_\mathcal{A} \langle s|\lambda \\ P_\mathcal{A} \lambda |s\rangle & P_\mathcal{A} \otimes \lambda^2 \end{pmatrix}. \tag{3.8}$$

This only adds a part to its null space and makes the notation in the next section somewhat simpler.

4. The Bloch–Floquet decomposition

In the previous sections $\chi(\boldsymbol{x}, t)$ is quite general but now we make the restriction to the spatially periodic case

$$\chi(\boldsymbol{x}, t) = \chi(\boldsymbol{x} + \boldsymbol{a}_j, t) \qquad j = 1, 2, 3 \tag{4.1}$$

where the $\boldsymbol{a}_j$ are nonvanishing and linearly independent in $\mathbb{R}^3$. Then also $\sigma(\boldsymbol{x}, \lambda) = \sigma(\boldsymbol{x} + \boldsymbol{a}_j, \lambda)$. From now on we shall assume that we have the situation as discussed in the previous section, i.e. $\chi(\boldsymbol{x}, t)$ is constant over $\mathcal{A}$. With $\mathcal{A}_0$ we shall indicate the restriction

$\mathcal{A} \cap \mathcal{C}_0$ of $\mathcal{A}$ to the unit cell $\mathcal{C}_0$ in coordinate space and with $\mathcal{B}$ the first Brillouin zone in the reciprocal space (see almost any text on solid state physics and, for a mathematically oriented discussion, [14]). In order to avoid technical problems we assume that $\mathcal{A}_0$ has a smooth boundary $\partial_{\mathcal{A}_0}$ (other situations and even fractal-shaped $\mathcal{A}_0$ can be handled as limits of smooth ones using a method discussed in [15]). We now make a Bloch decomposition of $\mathcal{H}_e$,

$$\mathcal{H}_e = \int_{\mathcal{B}}^{\oplus} \mathrm{d}\boldsymbol{k}\, \mathcal{H}' \tag{4.2}$$

where $\boldsymbol{k} \in \mathcal{B}$ and, with $\mathcal{H}_1' = L^2(\mathcal{C}_0, \mathrm{d}\boldsymbol{x}; \mathbb{C}^3)$, $\mathcal{H}_2' = \mathcal{H}_1' \otimes L^2(\mathbb{R}, \mathrm{d}\lambda)$, $\mathcal{H}' = \mathcal{H}_1' \oplus \mathcal{H}_2' = \mathcal{H}_1' \otimes \{\mathbb{C} \oplus L^2(\mathbb{R}, \mathrm{d}\lambda)\}$. Then

$$\mathsf{H}_e = \int_{\mathcal{B}}^{\oplus} \mathrm{d}\boldsymbol{k}\, \mathsf{H}_e(\boldsymbol{k}) \qquad [z^2 - \mathsf{H}_e]^{-1} = \int_{\mathcal{B}}^{\oplus} \mathrm{d}\boldsymbol{k}\, [z^2 - \mathsf{H}_e(\boldsymbol{k})]^{-1} \qquad \text{etc.} \tag{4.3}$$

Here $\mathsf{H}_e(\boldsymbol{k})$, which acts in $\mathcal{H}'$, is given by

$$\mathsf{H}_e(\boldsymbol{k}) = \begin{pmatrix} \mathsf{H}_0(\boldsymbol{k}) + P_0\|n\|_1 & P_0\langle s|\lambda \\ P_0\lambda|s\rangle & P_0 \otimes \lambda^2 \end{pmatrix} \tag{4.4}$$

where $P_0 = P_{\mathcal{A}_0}$ is the projector defined by $\Psi_{\mathcal{A}_0}(\boldsymbol{x})$.

We recall that in the Schrödinger case the functions in the domain of $\boldsymbol{p}^2(\boldsymbol{k})$ in $L^2(\mathcal{C}_0, \mathrm{d}\boldsymbol{x})$ have to satisfy the boundary conditions

$$f(\boldsymbol{x} + \boldsymbol{a}_j) = \exp[\mathrm{i}\theta_j] f(\boldsymbol{x}) \qquad \partial_x f(\boldsymbol{x} + \boldsymbol{a}_j) = \exp[\mathrm{i}\theta_j] \partial_x f(\boldsymbol{x}) \tag{4.5}$$

where $\theta_j \in [0, 2\pi)$ and $\boldsymbol{\theta}$ and $\boldsymbol{k}$ are related by (the $\boldsymbol{e}_j$ are the unit vectors along the three Cartesian axes in coordinate space)

$$\boldsymbol{M} \cdot \boldsymbol{\theta} = 2\pi\boldsymbol{k} \qquad \boldsymbol{e}_j = \boldsymbol{a}_j \cdot \boldsymbol{M}. \tag{4.6}$$

Noting that $\boldsymbol{p}^2(\boldsymbol{k})$ is in essence the differential operator $-\partial_x^2$, subject to the boundary conditions (4.5), its eigenvectors $\varphi_n(\boldsymbol{x}, \boldsymbol{k})$ and eigenvalues $\lambda_n^2(\boldsymbol{k})$ are given by

$$\varphi_n(\boldsymbol{x}, \boldsymbol{k}) = (2\pi)^{-3/2} \exp[\mathrm{i}(\boldsymbol{k} + \boldsymbol{k}_n) \cdot \boldsymbol{x}] \qquad \lambda_n^2(\boldsymbol{k}) = (2\pi)^2(\boldsymbol{k} + \boldsymbol{k}_n)^2 \qquad \boldsymbol{n} \in \mathbb{Z}^3 \tag{4.7}$$

where $\boldsymbol{k}_n = \boldsymbol{M} \cdot \boldsymbol{n}$. Note also that $[z - \boldsymbol{p}^2(\boldsymbol{k})]^{-1}$ is Hilbert–Schmidt for z outside the spectrum of $\boldsymbol{p}^2(\boldsymbol{k})$.

For $\mathsf{H}_0(\boldsymbol{k})$ in $\mathcal{H}_1'$ the situation is slightly different. Its null space $\mathcal{N}_0(\boldsymbol{k}) = P^{\|}(\boldsymbol{k})\mathcal{H}_1'$ is spanned by the functions $\{(2\pi)^{-3/2}\boldsymbol{e}_{k+k_n} \exp[\mathrm{i}(\boldsymbol{k} + \boldsymbol{k}_n) \cdot \boldsymbol{x}] = -\mathrm{i}\partial_x\varphi_n(\boldsymbol{x}, \boldsymbol{k})|\boldsymbol{n} \in \mathbb{Z}^3\}$. Since the $\varphi_n(\boldsymbol{x}, \boldsymbol{k})$ constitute an orthonormal basis for $L^2(\mathcal{C}_0, \mathrm{d}\boldsymbol{x})$ for any fixed $\boldsymbol{k} \in \mathcal{B}$, their closed linear span is $L^2(\mathcal{C}_0, \mathrm{d}\boldsymbol{x})$ itself and it will be clear that $\mathcal{N}_0(\boldsymbol{k})$ and $P^{\|}(\boldsymbol{k})$ do not depend on $\boldsymbol{k}$ and we can drop $\boldsymbol{k}$ in these objects. Then also $P^{\perp} = 1 - P^{\|}(\boldsymbol{k}) = 1 - P^{\|}$ does not depend on $\boldsymbol{k}$. Note that we introduced $P^{\perp}$ and $P^{\|}$ at an earlier stage but no confusion will arise by using the same notation for their Bloch-decomposed counterparts. However, the functions $\boldsymbol{f}(\boldsymbol{x})$ from the domain of $\mathsf{H}_0^{\perp}$, the restriction of H_0 to $P^{\perp}\mathcal{H}_1'$, have to satisfy the $\boldsymbol{k}$-dependent boundary conditions

$$\boldsymbol{f}(\boldsymbol{x} + \boldsymbol{a}_j) = \exp[\mathrm{i}\theta_j]\boldsymbol{f}(\boldsymbol{x}) \qquad \partial_x\boldsymbol{f}(\boldsymbol{x} + \boldsymbol{a}_j) = \exp[\mathrm{i}\theta_j]\partial_x\boldsymbol{f}(\boldsymbol{x}) \tag{4.8}$$

and the eigenvectors and eigenvalues associated with $\mathsf{H}_0^{\perp}$ are

$$\begin{aligned} \boldsymbol{\varphi}_{nj}(\boldsymbol{x}, \boldsymbol{k}) &= (2\pi)^{-3/2}\boldsymbol{u}_{nj} \exp[\mathrm{i}(\boldsymbol{k} + \boldsymbol{k}_n) \cdot \boldsymbol{x}] \\ \lambda_n^2(\boldsymbol{k}) &= (2\pi)^2(\boldsymbol{k} + \boldsymbol{k}_n)^2 \qquad \boldsymbol{n} \in \mathbb{Z}^3 \end{aligned} \tag{4.9}$$

where $\boldsymbol{k}_n = \boldsymbol{M} \cdot \boldsymbol{n}$ and the $\boldsymbol{u}_{nj}$ are two orthogonal unit vectors (polarization vectors) both orthogonal to $\boldsymbol{k} + \boldsymbol{k}_n$. We note further that in

$$[z^2 - \mathsf{H}_0(\boldsymbol{k})]^{-1} = z^{-2}P^{\|} + [z^2 - \boldsymbol{p}^2(\boldsymbol{k})]^{-1}P^{\perp} \tag{4.10}$$

$[z^2 - p^2(k)]^{-1}$ is compact (actually Hilbert–Schmidt) on $P^\perp \mathcal{H}_1$ but, since $P^\parallel$ is infinite dimensional, $[z^2 - \mathsf{H}_0(k)]^{-1}$ on $\mathcal{H}_1$ is not. This makes a further analysis significantly more complicated than in the Schrödinger case. Projecting $[z^2 - \mathsf{H}_e(k)]^{-1}$ upon $\mathcal{H}_1'$, we obtain

$$P_1[z^2 - \mathsf{H}_e(k)]^{-1}P_1 = \mathsf{R}_e(z, k)P_1 \tag{4.11}$$

where

$$\mathsf{R}_e(z, k) = [z^2 \varepsilon(x, z) - \mathsf{H}_0(k)]^{-1} = [z^2\{1 + P_0\hat{g}(z)\} - \mathsf{H}_0(k)]^{-1} \tag{4.12}$$

acting in $\mathcal{H}_1'$, is analytic in the open upper half plane. We want to know whether or not it has a limit as $\text{Im}\, z \downarrow 0$. First we check the invertibility of $\lambda^2 \varepsilon(x, \lambda) - \mathsf{H}_0(k)$ for real, non-zero λ.

Proposition 4.1. *Let $\lambda \in \mathbb{R}$, $\lambda \neq 0$, and suppose*

$$\text{Im}\, \hat{g}(\lambda) = \frac{\pi}{\lambda}n(\lambda) \neq 0. \tag{4.13}$$

Then

$$[\lambda^2 \varepsilon(x, \lambda) - \mathsf{H}_0(k)] \cdot f = 0 \qquad f \in \mathcal{D}(\mathsf{H}_0(k)) \tag{4.14}$$

has no solutions for any $k \in \mathcal{B}$, i.e. the null space of $\lambda^2 \varepsilon(x, \lambda) - \mathsf{H}_0(k)$ is empty for any $k \in \mathcal{B}$.

Proof. Taking the inner product of (4.14) with f we have

$$([\lambda^2 \varepsilon(x, \lambda) - \mathsf{H}_0(k)] \cdot f, f) = 0.$$

Its imaginary part is

$$\pi \lambda n\,(\lambda)(\Psi_{\mathcal{A}_0}(x)f, f) = 0$$

implying that $f(x) = 0$ for $x \in \mathcal{A}_0$. Then, since $\varepsilon(x, \lambda) = 1$ for $x \notin \mathcal{A}_0$,

$$([\lambda^2 - \mathsf{H}_0(k)] \cdot f(x)) = 0 \qquad x \notin \mathcal{A}_0.$$

Since $\lambda \neq 0$ this implies that $P^\parallel f(x) = 0$ for $x \notin \mathcal{A}_0$. However, $f(x)$ vanishes on $\mathcal{A}_0$ so $P^\parallel f(x) = 0$ on $\mathcal{C}_0$, i.e. $f(x)$ is transverse and (4.14) reduces to

$$[\lambda^2 - p(k)^2]f(x) = 0 \qquad x \notin \mathcal{A}_0.$$

The solutions are given by (4.9), i.e.,

$$f(x) = \sum_{n \in \mathbb{Z}^3} \sum_j a_{nj}\varphi_n(x, k) = \sum_{n \in \mathbb{Z}^3} \sum_j a_{nj}(2\pi)^{-3/2}u_{nj}\exp[i(k + k_n) \cdot x]$$

where the sum over n is restricted according to $\lambda^2 = (k + k_n)^2$ and hence is finite. For given λ there are either no solutions or a finite sum over n. In the latter case continuity requires $f(x)$ and $\partial_x \times f(x)$ to vanish on the boundary $\partial_{\mathcal{A}_0}$ of $\mathcal{A}_0$ implying that $f = 0$. $\qquad \square$

Note that the situation is different in the conservative case and also if $n(\lambda) = 0$ in some open interval $\Delta \subset \mathbb{R}$. In the latter case $\text{Im}\, \hat{g}(\lambda) = 0$ for $\lambda \in \Delta$, but

$$\text{Re}\, \hat{g}(\lambda) = \int d\omega\, n(\omega)[\omega^2 - \lambda^2]^{-1} \qquad \lambda \in \Delta \tag{4.15}$$

need not vanish and we have a non-trivial dispersive situation, i.e. for $x \in \mathcal{A}_0$ and $\omega \in \Delta$, $\varepsilon(x, \omega)$ is a real, non-constant function of ω.

Proposition 4.2. *Let $\lambda \in \mathbb{R}$, $\lambda \neq 0$ and $n(\lambda) = 0$. Then the solutions $f_{\lambda j}$ of*

$$[\lambda^2 \varepsilon(x, \lambda) - \mathsf{H}_0(k)] \cdot f_{\lambda j} = 0 \qquad f_{\lambda j} \in \mathcal{D}(\mathsf{H}_0(k)) \tag{4.16}$$

span a finite-dimensional subspace $\mathcal{H}_\lambda = P_\lambda \mathcal{H}$.

Proof. Dismissing the trivial case that (4.16) has no solutions, we have

$$\lambda^2 \varepsilon(\boldsymbol{x}, \lambda) P^\| \boldsymbol{f}_{\lambda j} + [\lambda^2 \varepsilon(\boldsymbol{x}, \lambda) - \boldsymbol{p}(\boldsymbol{k})^2] P^\perp \boldsymbol{f}_{\lambda j} = 0.$$

However, since $\varepsilon(\boldsymbol{x}, \lambda)$ is constant outside the interface ∂_{A_0}, it follows that $\boldsymbol{f}_{\lambda j}(\boldsymbol{x})$ is transverse outside this boundary and consequently $P^\| \boldsymbol{f}_{\lambda j} = 0$. For given λ we can take the $\boldsymbol{f}_{\lambda j}$s orthonormal and define $P_\lambda = \sum_j | \boldsymbol{f}_{\lambda j} \rangle \langle \boldsymbol{f}_{\lambda j} |$. Then

$$[\lambda^2 \varepsilon(\boldsymbol{x}, \lambda) - \boldsymbol{p}(\boldsymbol{k})^2] P_\lambda = 0$$

or, with $a > 0$,

$$[\boldsymbol{p}(\boldsymbol{k})^2 + a] P_\lambda = [\lambda^2 \varepsilon(\boldsymbol{x}, \lambda) + a] P_\lambda$$

so, since $\boldsymbol{p}(\boldsymbol{k})^2 \geqslant 0$,

$$P_\lambda = [\boldsymbol{p}(\boldsymbol{k})^2 + a]^{-1} [\lambda^2 \varepsilon(\boldsymbol{x}, \lambda) + a] P_\lambda$$

and ($\|\lambda^2 \varepsilon(\boldsymbol{x}, \lambda) + a\|$ is the operator norm of $\lambda^2 \varepsilon(\boldsymbol{x}, \lambda) + a$),

$$\operatorname{tr} P_\lambda = \operatorname{tr} P_\lambda^* P_\lambda = \operatorname{tr} P_\lambda [\lambda^2 \varepsilon(\boldsymbol{x}, \lambda) + a][\boldsymbol{p}(\boldsymbol{k})^2 + a]^{-2} [\lambda^2 \varepsilon(\boldsymbol{x}, \lambda) + a] P_\lambda$$
$$\leqslant \|\lambda^2 \varepsilon(\boldsymbol{x}, \lambda) + a\|^2 \operatorname{tr} [\boldsymbol{p}(\boldsymbol{k})^2 + a]^{-2} < \infty$$

since $[\boldsymbol{p}(\boldsymbol{k})^2 + a]^{-1}$ is Hilbert–Schmidt. $\qquad \square$

Remark. Solutions $\boldsymbol{f}_{\lambda j}$ for different λ are in general not orthonormal but satisfy a more complicated relation, see section 7.2.

5. Consequences of analyticity

We start by introducing some notation. Thus $\Gamma(\psi) = \exp[\mathrm{i}\psi]\overline{\mathbb{R}}^+$, and, for $\psi > 0$, $\mathcal{S}(-\psi) = \{z \in \mathbb{C} | z \neq 0, \arg z \in (-\psi, 0)\}$, $\mathcal{S}(\psi) = \{z \in \mathbb{C} | z \neq 0, \arg z \in (0, \psi)\}$ and $\mathcal{S}(|\psi|) = \{z \in \mathbb{C} | z \neq 0, |\arg z| < \psi\}$. We note that

$$\hat{g}(z) = \int_{-\infty}^{+\infty} \mathrm{d}\lambda \, n(\lambda)[\lambda^2 - z^2]^{-1} = 2 \int_0^{+\infty} \mathrm{d}\lambda \, n(\lambda)[\lambda^2 - z^2]^{-1} \tag{5.1}$$

is positive for z on the positive imaginary axis and has a positive imaginary part for z in the open first quadrant and a negative one in the open second one. Our aim is to make use of an analytic continuation of $\hat{g}(z)$ across the real axis. This can be achieved by making one of the following assumptions.

A_4: There exists an $\alpha > 0$ such that

$$\int_0^\infty \mathrm{d}t \, \exp[\alpha|t|]|g'(t)| \leqslant c_4 < \infty. \tag{5.2}$$

Since

$$n(\lambda) = \pi^{-1} \int_0^\infty \mathrm{d}t \, \cos \lambda t g'(t) \tag{5.3}$$

it now follows that $n(\lambda)$ has an analytic continuation into the strip $\{z \in \mathbb{C} | \, |\operatorname{Im} z| < \alpha\}$ and also that $\hat{g}(z)$ is analytic in $\{z \in \mathbb{C} | \operatorname{Im} z > -\alpha\}$.

A_5: There exists a $\beta > 0$ such that $g'(t)$, $t \geqslant 0$, has an analytic continuation into the sector $S(|\beta|)$ and

$$\int_0^\infty \mathrm{d}t \, |g'(t \exp[\mathrm{i}\psi])| \leqslant c_5 < \infty \qquad |\psi| < \beta. \tag{5.4}$$

Now $n(\lambda)$ can be continued into $S(|\beta|)$. Also $\hat{g}(z)$ (which is already analytic in $\mathbb{C}^+$) has a continuation into $S(-\beta)$. In particular, starting with $\operatorname{Im} z > 0$, by contour deformation,

$$
\begin{aligned}
\hat{g}(z) &= 2\int_0^\infty d\lambda\,[\lambda^2 - z^2]^{-1} n(\lambda) = 2\int_{\Gamma(-\psi)} d\lambda\,[\lambda^2 - z^2]^{-1} n(\lambda) \\
&= 2e^{i\psi}\int_0^\infty d\lambda\,[\lambda^2 e^{2i\psi} - z^2]^{-1} n(\lambda e^{i\psi}) \\
&= 2\int_0^\infty d\lambda\,[\lambda^2 - z^2 e^{-2i\psi}]^{-1} n(\lambda e^{i\psi})
\end{aligned}
\tag{5.5}
$$

where $|\psi| < \beta$. Taking $\psi > 0$ we can now continue across $\mathbb{R}^+$.

A_6: $n(\lambda)$, $\lambda > 0$, has an analytic continuation into the open set $\mathcal{N}^+ \supset \mathbb{R}^+$, symmetric with respect to $\mathbb{R}$, and containing a non-trivial interval $\Delta \subset \mathbb{R}^+$ on which it is not constant.

Thus, with Γ a contour obtained by deforming $\mathbb{R}^+$ locally into $\mathbb{C}^- \cap \mathcal{N}^+$ and back,

$$
\hat{g}(z) = 2\int_0^\infty d\lambda\,[\lambda^2 - z^2]^{-1} n(\lambda) = 2\int_\Gamma d\lambda\,[\lambda^2 - z^2]^{-1} n(\lambda) \qquad z \in \mathbb{C}^+
\tag{5.6}
$$

and $\hat{g}(z)$ can now be continued across $\mathbb{R}^+$ into $\mathbb{C}^- \cap \mathcal{N}^+$. For such z, by closing the contour and picking up the residue in z, we then have

$$
\hat{g}(z) = 2\int_0^\infty d\lambda\,[\lambda^2 - z^2]^{-1} n(\lambda) + 2\pi i z^{-1} n(z) \qquad z \in \mathbb{C}^- \cap \mathcal{N}^+
\tag{5.7}
$$

where the first term can be continued throughout $\mathbb{C}^-$ but the second is restricted to the analyticity domain of $n(z)$. Since $n(\lambda) = n(-\lambda)$ there is also a continuation of $n(\lambda)$ into $\mathcal{N}^- = \{-z | z \in \mathcal{N}^+\}$ and we denote $\mathcal{N} = \mathcal{N}^+ \cup \mathcal{N}^-$. In certain cases, such as A_4, $n(\lambda)$ can actually be continued into $\mathcal{N} \supset \mathbb{R}$. Next we note that $n(\lambda)$ cannot be constant on any real interval since then it must be constant throughout $\mathbb{R}$ and this is in conflict with $\|n\|_1$ being finite. In particular the set $\Lambda = \{\lambda \in \mathbb{R} | n(\lambda) = 0, \lambda \neq 0\}$ of zeros of $n(\lambda)$ is discrete. A_4 and A_5 are easily checked for specific models (an example is given in section 8) and both imply A_6. A_4 requires exponential decay of $g'(t)$ and A_5 does not. Instead it involves some analyticity properties and allows the use of the powerful complex dilatation method, to be discussed later.

Assuming A_6, then, if $n(\lambda_0) > 0$ for some $0 \neq \lambda_0 \in \mathcal{N}$, it follows that $|\operatorname{Im} \hat{g}(z)| \geqslant c > 0$ in an open neighbourhood $\mathcal{U}_\delta(\lambda_0)$ of λ_0. Hence, according to proposition 4.1, $R_e(\lambda^2, \boldsymbol{k})$ exists for $\lambda \in \Delta = \mathcal{U}_\delta(\lambda_0) \cap \mathbb{R}$ but it need not be bounded nor do we know whether or not it is the limit of $R_e(z, \boldsymbol{k})$. To investigate this further we return to

$$
R_e(z, \boldsymbol{k}) = [z^2 \varepsilon(\boldsymbol{x}, z) - H_0(\boldsymbol{k})]^{-1} = [z^2\{1 + P_0\hat{g}(z)\} - H_0(\boldsymbol{k})]^{-1}.
\tag{5.8}
$$

We know from proposition 2.3 that it is analytic in the open upper half plane. Here we want to exploit the tandem of compactness and analyticity in order to obtain information about its analytic continuation into $\mathbb{C}^-$. However, the fact that $H_0(\boldsymbol{k})$ has an infinite-dimensional null space complicates the situation. We therefore isolate the offending part by once more using the Feshbach formula. Writing $P = P^\perp$, $Q = P^\parallel$, it gives

$$
\begin{aligned}
R_e(z, \boldsymbol{k}) &= [z^2 \varepsilon(\boldsymbol{x}, z) - H_0(\boldsymbol{k})]^{-1} \\
&= z^{-2} Q[Q\varepsilon(\boldsymbol{x}, z)Q]^{-1}Q + \{P + Q[Q\varepsilon(\boldsymbol{x}, z)Q]^{-1}Q\varepsilon(\boldsymbol{x}, z)P\} \\
&\quad \times \mathcal{G}(z)\{P + P\varepsilon(\boldsymbol{x}, z)Q[Q\varepsilon(\boldsymbol{x}, z)Q]^{-1}Q\}
\end{aligned}
\tag{5.9}
$$

where

$$
\begin{aligned}
\mathcal{G}(z) &= P[z^2 \varepsilon(\boldsymbol{x}, z) - H_0(\boldsymbol{k})]^{-1} P \\
&= [z^2\{P\varepsilon(\boldsymbol{x}, z)P + P\varepsilon(\boldsymbol{x}, z)Q[Q\varepsilon(\boldsymbol{x}, z)Q]^{-1}Q\varepsilon(\boldsymbol{x}, z)P\} - \boldsymbol{p}^2(\boldsymbol{k})]^{-1} P \\
&= [z^2\{P\varepsilon(\boldsymbol{x}, z)P + P\hat{\chi}(\boldsymbol{x}, z)Q[Q\varepsilon(\boldsymbol{x}, z)Q]^{-1}Q\hat{\chi}(\boldsymbol{x}, z)P\} - \boldsymbol{p}^2(\boldsymbol{k})]^{-1} P \\
&= [z^2 P[P\varepsilon(\boldsymbol{x}, z)^{-1}P]^{-1}P - \boldsymbol{p}^2(\boldsymbol{k})]^{-1} P.
\end{aligned}
\tag{5.10}
$$

$\mathcal{G}(z)$ is a serious candidate for compactness since $[z^2 - p^2(k)]^{-1}$ has this property outside the eigenvalues of $p^2(k)$. However, we first have to ascertain that the operators $Q[Q\varepsilon(x, z)Q]^{-1}Q$ and $P[P\varepsilon(x, z)^{-1}P]^{-1}P$ make sense.

Definition 5.1. *Let $\mathcal{D}$ be the analyticity domain of $\hat{g}(z)$ and let $\mathcal{V} = \{z \in \mathcal{D}|\hat{g}(z) \in (-\infty, -1)\}$. Since* $\operatorname{Im} \hat{g}(z) = 0$ *on $\mathcal{V}$, it follows that 0 and $\mathbb{C}^+$ are not in $\mathcal{V}$, whereas other real elements of $\mathcal{V}$ must be contained in the set Λ. Moreover $\mathcal{V}$ is closed in $\mathcal{D}$, so $\mathcal{Z} = \mathcal{D}\backslash\mathcal{V}$ is open.*

Lemma 5.2. $Q[Q\varepsilon(x, z)Q]^{-1}Q$ *and* $P[P\varepsilon(x, z)^{-1}P]^{-1}P$ *exist as bounded operators for $z \in \mathcal{Z}$ and are analytic on $\mathcal{Z}$.*

Proof. Denoting $P_0 = P_{\mathcal{A}_0}$ as before, $Q_0 = 1 - P_0$, we have

$$\varepsilon(x, z) = 1 + \hat{g}(z)P_0 = Q_0 + \{1 + \hat{g}(z)\}P_0$$

leading to

$$\varepsilon(x, z)^{-1} = Q_0 + [1 + \hat{g}(z)]^{-1}P_0 = [1 + \hat{g}(z)]^{-1}\{1 + \hat{g}(z)Q_0\}.$$

Now

$$Q\varepsilon(x, z)Q = Q + \hat{g}(z)M \qquad M = QP_0Q$$

so, on $Q\mathcal{H}_1$, we are dealing with the inverse of $1 + \hat{g}(z)M$,

$$Q[Q\varepsilon(x, z)Q]^{-1}Q = Q[1 + \hat{g}(z)M]^{-1}Q = \hat{g}(z)^{-1}[\hat{g}(z)^{-1} - (-M)]^{-1}Q.$$

Noting that $-M$ has spectrum in $[-1, 0]$, it follows that it exists as a bounded-operator-valued analytic function of $z \in \mathcal{Z}$. Next

$$P\varepsilon(x, z)^{-1}P = [1 + \hat{g}(z)]^{-1}\{P + \hat{g}(z)N\}$$
$$= \hat{g}(z)[1 + \hat{g}(z)]^{-1}[\hat{g}(z)^{-1}P + N] \qquad N = PQ_0P$$

and

$$P[P\varepsilon(x, z)^{-1}P]^{-1}P = \hat{g}(z)^{-1} = [1 + \hat{g}(z)]P[1 + \hat{g}(z)N]^{-1}P$$

which again exists as a bounded-operator-valued analytic function of $z \in \mathcal{Z}$. $\square$

Theorem 5.3. *Suppose that A_1–A_2 and A_6 hold. Then $\mathsf{R}_e(z, k)$ can be continued as a meromorphic function into $\mathbb{C}^- \cap \mathcal{Z}$, where it can have poles $\lambda_r(k)$ with finite-dimensional associated residues $\mathsf{A}_r(k)$. In addition it has a pole with infinite-dimensional residue in $z = 0$ and it can have poles in the set Λ, in which case the residues are finite-dimensional projectors. In particular $\mathsf{R}_e(z, k)$ and $\mathsf{R}_e(z)$ have a non-vanishing limit as a bounded operator for $\delta \downarrow 0$ in $z = \lambda + i\delta$, $\lambda \in \mathbb{R} \cap \mathcal{Z}$.*

Proof. Noting that

$$z^2 P[P\varepsilon(x, z)^{-1}P]^{-1}P = z^2 P - z^2\hat{g}(z)[1 + \hat{g}(z)N]^{-1}\{N - 1\}P = z^2 P - W(z)P$$

where

$$W(z) = -z^2\hat{g}(z)[1 + \hat{g}(z)N]^{-1}\{1 - N\}P$$

we have, omitting obvious P,

$$\mathcal{G}(z) = [z^2 - p(k)^2 - W(z)]^{-1} = R_0(z)[1 - K(z)]^{-1}$$

with

$$R_0(z) = [z^2 - p(k)^2]^{-1} \qquad K(z) = W(z)R_0(z).$$

$R_0(z)$ is compact analytic on $P\mathcal{H}_1$ for $z \in \mathcal{Z}$, except for the intersection $\mathcal{Z}' = \mathcal{Z} \cap \sigma(p(k)^2)$, where $\sigma(p(k)^2)$ is the discrete set of eigenvalues of $p(k)^2$, and hence the same is true for $K(z)$. It then follows from the analytic Fredholm theorem that $\mathcal{G}(z)$, $z \in \mathcal{Z}'$, can only have poles with associated finite-dimensional residues and the same applies to $R_e(z, k)$, all other terms in (5.9) being analytic on $\mathcal{Z}$. However, as we have shown in section 4, the equation

$$[\lambda^2 \varepsilon(x, \lambda) - H_0(k)] \cdot f = 0 \qquad 0 \neq \lambda \in \mathbb{R} \tag{5.11}$$

can only have solutions in λ with Im $\hat{g}(\lambda) = 0$, i.e. for $\lambda \in \Lambda$, in which case proposition 4.2 applies. It follows that $R_e(z, k)$ has a non-vanishing limit as a bounded operator for $\delta \downarrow 0$ in $z = \lambda + i\delta$, $\lambda \in \mathbb{R} \cap \mathcal{Z}$ and this limit is non-zero by analyticity. Since $\mathcal{Z}$ does not depend on k this result extends to $R_e(z)$. $\qquad \square$

Note that not all of the assumptions A_1 and A_2 are necessary to arrive at the stated result. In addition we note that the exclusion of the set $\mathcal{V}$ from $\mathcal{D}$ was done for technical reasons and it is not impossible that it can be avoided, using different techniques.

Corollary 5.4. *Under the assumptions of theorem 5.3, $R_e(z, k)$ has the representation*

$$R_e(z, k) = z^{-1} A_0 + \sum_{r \neq 0} [z - \lambda_r(k)]^{-1} A_r(k) + R_e'(z, k) \qquad z \in \mathcal{Z} \cup \Lambda \tag{5.12}$$

with $R_e'(z, k)$ analytic on $\mathcal{Z} \cup \Lambda$. The $A_r(k)$, $r \neq 0$, are finite dimensional and A_0 and those $A_r(k)$, $r \neq 0$, with $\lambda_r(k)$ real, are mutually orthogonal projectors.

Next we obtain one of the main results of this paper.

Corollary 5.5. *A system satisfying A_1, A_2 and A_6 does not have bandgaps.*

Proof. According to (2.20)

$$\tilde{E}(\omega) = 2\pi\omega \int_{\mathcal{B}}^{\oplus} dk\, R_e(\omega - i0, k) P_0 n(\omega) R_e(\omega + i0, k)\{i\omega E(0) - \partial_x \times B(0)\}$$

$$= 2\pi\omega n(\omega) \int_{\mathcal{B}}^{\oplus} dk\, R_e(\omega - i0, k) P_0 R_e(\omega + i0, k)\{i\omega E(0) - \partial_x \times B(0)\}. \tag{5.13}$$

For $\omega \in \mathbb{R} \cap \mathcal{Z}$, $R_e(\omega + i0, k)$ and $R_e(\omega - i0, k) = R_e(\omega + i0, k)^*$ exist and are non-zero, whereas $n(\omega)$ is strictly positive. According to proposition 4.1, $R_e(\omega + i0, k)$ has dense range in $\mathcal{H}_1$ for any $k \in \mathcal{B}$, whereas the null space of P_0 and the range of $R_e(\omega + i0, k)$ have zero intersection (see the proof of proposition 4.1). Hence

$$\int_{\mathcal{B}}^{\oplus} dk\, R_e(\omega - i0, k) P_0 R_e(\omega + i0, k)$$

is a strictly positive operator, so $\tilde{E}(\omega)$ cannot vanish for every $i\omega E(x, 0) - \partial_x \times B(x, 0) \in \mathcal{H}_1$. Since $\mathbb{R} \setminus (\mathbb{R} \cap \mathcal{Z})$ consists of discrete points, the statement is proven. $\qquad \square$

This result raises the question whether or not bandgaps can exist at all. This may indeed be the case if $n(\lambda)$ vanishes on an interval $\Delta = [a, b] \subset \mathbb{R}^+$. Then (5.13) can no longer be used for $\lambda \in \Delta$, since the resolvents need not have a limit. However, proposition 4.2 applies and the collection of eigenvalues $\{\lambda_r(k) | k \in \mathcal{B}\}$ may leave gaps in Δ, i.e. $\Delta \setminus \{\lambda_r(k) | k \in \mathcal{B}\}$ may contain one or more nontrivial intervals Δ_j. Then $R_e(z)$ can be analytic through Δ_j (at

this point we can only conclude that $z^2 \varepsilon(\boldsymbol{x}, z) - \mathsf{H}_0$ is invertible) in which case, according to the second line in (1.18), $\tilde{\boldsymbol{E}}(\omega)$ vanishes for $\omega \in \Delta_j$. A proper analysis could start from the observation that, although A_6 no longer holds, $\hat{g}(z)$ can still be continued into $\mathbb{C}^-$, since now

$$\hat{g}(z) = 2 \int_0^a \mathrm{d}\lambda \, [\lambda^2 - z^2]^{-1} n(\lambda) + 2 \int_b^\infty \mathrm{d}\lambda \, [\lambda^2 - z^2]^{-1} n(\lambda) \tag{5.14}$$

allowing a continuation from $\mathbb{C}^+$ into $\mathbb{C}^-$ through (a, b) and $(-b, -a)$. Generically $\hat{g}(x)$ ranges through all of $\mathbb{R}$ as x ranges through $[a, b]$ and there will be a subinterval $\Delta' = (b - \delta, b]$ left that is not contained in $\mathcal{V}$. Then the previous analysis can be applied but we do not have control over the limit of $\mathsf{R}_e(z, \boldsymbol{k})$ as z approaches $\mathbb{R}$ outside Δ'.

6. Resonances associated with H_e

6.1. Complex dilatation basics

In $\mathsf{H}_e(\boldsymbol{k})$ the operators $\mathsf{H}_0(\boldsymbol{k})$, with discrete spectrum in $\mathbb{R}^+$ and $P_0 \otimes \lambda^2$, which has $\overline{\mathbb{R}}^+$ as its (absolutely continuous) spectrum, are coupled and we expect that this causes the eigenvalues of $\mathsf{H}_0(\boldsymbol{k})$ to turn into resonances, i.e. they acquire an imaginary part. Resonances can often be uncovered as eigenvalues or poles in an analytic continuation in another Riemann sheet. To do so a procedure is needed that makes such a continuation possible and in this section we exploit the idea to use a complex dilatation [14, 16] in the λ-variable to disentangle the spectrum of λ^2 from the spectrum of $\mathsf{H}_0(\boldsymbol{k})$ in H_e. Then the eigenvalues of the latter become isolated and perturbation theory can be used for their calculation. Thus we define on $\mathcal{H}_2$ the group of unitary operators $\{U_2(\vartheta) | \vartheta \in \mathbb{R}\}$ through

$$U_2(\vartheta) \boldsymbol{f}(\boldsymbol{x}, \lambda) = \mathrm{e}^{-\frac{\vartheta}{2}} \boldsymbol{f}(\boldsymbol{x}, \mathrm{e}^{-\vartheta} \lambda) \qquad \boldsymbol{f} \in \mathcal{H}_2 \tag{6.1}$$

and extend it to $\mathcal{H}'$ according to

$$U_d(\vartheta) = \begin{pmatrix} 1 & 0 \\ 0 & U_2(\vartheta) \end{pmatrix}. \tag{6.2}$$

Then, writing,

$$\mathsf{H}_e(\boldsymbol{k}) = \begin{pmatrix} \mathsf{H}_0(\boldsymbol{k}) + \|n\|_1 P_0 & P_0 \langle s | \lambda \\ P_0 \lambda | s \rangle & P_0 \otimes \lambda^2 \end{pmatrix} = \mathsf{H}_e^{(0)}(\boldsymbol{k}) + \mathsf{V} \tag{6.3}$$

where

$$\mathsf{H}_e^{(0)}(\boldsymbol{k}) = \begin{pmatrix} \mathsf{H}_0(\boldsymbol{k}) & 0 \\ 0 & P_0 \otimes \lambda^2 \end{pmatrix} \qquad \mathsf{V} = \begin{pmatrix} \|n\|_1 P_0 & P_0 \langle s | \lambda \\ P_0 \lambda | s \rangle & 0 \end{pmatrix} \tag{6.4}$$

we have

$$\mathsf{H}_e^{(0)}(\boldsymbol{k}, \vartheta) \equiv U_d(\vartheta) \mathsf{H}_e^{(0)}(\boldsymbol{k}) U_d^{-1}(\vartheta) = \begin{pmatrix} \mathsf{H}_0(\boldsymbol{k}) & 0 \\ 0 & \lambda^2 \mathrm{e}^{-2\vartheta} P_0 \end{pmatrix}. \tag{6.5}$$

Setting $u(\lambda) = \lambda s(\lambda)$,

$$U_d(\vartheta) u(\lambda) = u(\lambda, \vartheta) = \mathrm{e}^{-\vartheta/2} u(\mathrm{e}^{-\vartheta} \lambda) = \mathrm{e}^{-3/2\vartheta} \lambda s(\mathrm{e}^{-\vartheta} \lambda) \tag{6.6}$$

and

$$\mathsf{V}(\vartheta) = U_d(\vartheta) \mathsf{V} U_d^{-1}(\vartheta) = \begin{pmatrix} \|n\|_1 P_0 & P_0 \langle u(\vartheta) | \\ P_0 | u(\vartheta) \rangle & 0 \end{pmatrix}. \tag{6.7}$$

Here $\mathsf{H}_e^{(0)}(\boldsymbol{k}, \vartheta)$ has a spectrum on the positive real axis consisting of the absolutely continuous spectrum $\sigma_{\mathrm{ac}} = [0, \infty]$ of $\lambda^2 \mathrm{e}^{-2\vartheta} P_0$, overlayered with the eigenvalue zero (which has

infinite multiplicity) and the discrete eigenvalues λ_n (which have finite multiplicity) of $\mathsf{H}_0(\boldsymbol{k})$. However, after a complex dilatation,

$$\vartheta \to \zeta = \vartheta + \mathrm{i}\psi \tag{6.8}$$

$\mathsf{H}_e^{(0)}(\boldsymbol{k}, \vartheta)$ changes into

$$\mathsf{H}_e^{(0)}(\boldsymbol{k}, \zeta) = \begin{pmatrix} \mathsf{H}_0(\boldsymbol{k}) & 0 \\ 0 & P_0 \otimes \lambda^2 \mathrm{e}^{-2\zeta} \end{pmatrix} \tag{6.9}$$

where the absolutely continuous spectrum is rotated over -2ψ, i.e. $\sigma_{\mathrm{ac}} \to \sigma(\psi) = \exp[-2\mathrm{i}\psi]\overline{\mathbb{R}}^+$. Thus the spectrum of $\mathsf{H}_e^{(0)}(\boldsymbol{k}, \zeta)$ consists of σ_d, the isolated eigenvalues λ_n on the positive real axis, which have finite multiplicity, and the essential spectrum $\sigma_{\mathrm{ess}}(\zeta) = \exp[-2\mathrm{i}\psi]\overline{\mathbb{R}}^+$, i.e. the set $\sigma(\psi)$ (which contains the eigenvalue zero). We now assume that A$_1$–A$_3$ and A$_5'$ are satisfied, where

A$_5'$: The statements of A$_5$ hold and moreover $s(\lambda) = \sqrt{n(\lambda)}$ has an analytic continuation into $S(|\beta|)$.

Then $u(\vartheta)$ has an analytic continuation $u(\zeta)$ as a square integrable function of λ and

$$\mathsf{V}(\zeta) = \begin{pmatrix} \|n\|_1 P_0 & P_0\langle u(\bar{\zeta})| \\ P_0|u(\zeta)\rangle & 0 \end{pmatrix} \tag{6.10}$$

is well defined. Thus Rayleigh–Schrödinger perturbation theory can be used to obtain the new eigenvalues if $\mathsf{V}(\zeta)$ is applied. A simple calculation, to second order in V, shows that the perturbed eigenvalue originating from λ_n, apart from being shifted and possibly being split, acquires a negative imaginary part if $n(\lambda_n) > 0$. Note that low-order perturbation results need not be accurate in this case and different perturbation techniques may be required. The situation is similar to that of continuum-embedded eigenvalues in atoms, where the Coulomb repulsion between the electrons changes them into resonances (auto-ionizing states). Note further that the maximally allowed dilatation angle ψ follows from the assumed analyticity in A$_5$ and it may happen that a particular resonance cannot be uncovered. Finally we remark that the perturbed eigenvalues do not depend on ψ. A related matter is what happens with $\sigma_{\mathrm{ess}}(\zeta)$ as $\mathsf{V}(\zeta)$ is turned on. This will be discussed below.

6.2. Stability of the essential spectrum

In the Schrödinger case the stability of $\sigma_{\mathrm{ess}}(\zeta)$ is usually obtained by making use of the stability of essential spectrum under relatively compact perturbations [14, 16]. Thus, with $H = \boldsymbol{p}^2 + V(\boldsymbol{x})$ in $L^2(\mathbb{R}^3, \mathrm{d}\boldsymbol{x})$, V a real potential, it is shown that $K(z) = V[z - \boldsymbol{p}^2]^{-1}$ in $R(z) = [z - H]^{-1} = [z - \boldsymbol{p}^2]^{-1}[1 - K(z)]^{-1}$ is compact, usually by establishing that it is a Hilbert–Schmidt operator. Then a real dilatation, $\boldsymbol{x} \to \mathrm{e}^{\vartheta}\boldsymbol{x}$, is made, so $\boldsymbol{p} \to \mathrm{e}^{-\vartheta}\boldsymbol{p}$, $V(\boldsymbol{x}) \to V(\mathrm{e}^{\vartheta}\boldsymbol{x})$, $H \to H(\vartheta)$ and $K(z) \to K(z, \vartheta)$. Since this involves the unitary transformation

$$U_d(\vartheta) = \exp\left[\mathrm{i}\frac{\vartheta}{2}\{\boldsymbol{x} \cdot \boldsymbol{p} + \boldsymbol{p} \cdot \boldsymbol{x}\}\right] \tag{6.11}$$

nothing changes. Keeping z fixed in the upper half plane it is then possible to continue ϑ, $\vartheta \to \zeta = \vartheta + \mathrm{i}\psi$, $\psi > 0$. Provided V has the proper analyticity properties, $K(z, \zeta) = V(\zeta)[z - \mathrm{e}^{-2\zeta}\boldsymbol{p}^2]^{-1}$ remains compact and $R(z, \zeta) = [z - H(\zeta)]^{-1} = [z - \mathrm{e}^{-2\zeta}\boldsymbol{p}^2]^{-1}[1 - K(z, \zeta)]^{-1}$ can now be continued in z into the sector $\mathcal{S}(-2\psi)$ in the lower half plane. It then follows from the Fredholm theorem that the essential spectrum of $H(\zeta)$ coincides with that of $\mathrm{e}^{-2\zeta}\boldsymbol{p}^2$ (cf [16]). In addition to possible eigenvalues in $\mathbb{R}$, non-real eigenvalues

($H(\zeta)$ is no longer selfadjoint) in $\mathcal{S}(-2\psi)$ may be present, which can be calculated to leading order as discussed above.

In the Maxwell case the situation is more complicated for two reasons. The first is that $H_e(\boldsymbol{k})$ has an infinite-dimensional null space $\mathcal{N}$, which in addition depends on V. However, the null space can be projected out but then we run into the second problem, which is that the analogue of $K(z)$, above, is not compact. However, its square turns out to be Hilbert–Schmidt, which suffices for our purpose, as follows from $[1 - K(z)]^{-1} = [1 + K(z)][1 - K(z)^2]^{-1}$. We note that the tools at our disposal are the compactness of $[z^2 - \boldsymbol{p}^2(\boldsymbol{k})]^{-1}$ and the fact that in $V(\zeta)$ the objects $|u(\zeta)\rangle$ and $\langle u(\bar{\zeta})|$ lead to finite rank perturbations. As noted above the null space $\mathcal{N}$ depends on V and hence differs from $\mathcal{N}_0$, the null space of $H_e^{(0)}(\boldsymbol{k})$. This will now be remedied.

6.3. A unitary transformation

As discussed in the appendix, there exists a unitary transformation U with the property

$$\hat{H}_e(\boldsymbol{k}) = U^{-1}H_e(\boldsymbol{k})U$$
$$= \begin{pmatrix} H_0(\boldsymbol{k}) + \|n\|_1 P^\perp P_0 P^\perp & P^\perp P_0\{\|n\|_1 Z_0\langle\lambda^{-1}s| + \langle\lambda s|\} \\ \{\|n\|_1 Z_0|\lambda^{-1}s\rangle + |\lambda s\rangle\}P_0 P^\perp & P_0 \otimes \lambda^2 + Z_0 \otimes \{|\lambda s\rangle\langle\lambda^{-1}s| + |\lambda^{-1}s\rangle\langle\lambda s|\} + \|n\|_1 Z_0^2 \otimes |\lambda^{-1}s\rangle\langle\lambda^{-1}s| \end{pmatrix} \tag{6.12}$$

has $\mathcal{N}_0$ as its null space. Here

$$Z_0 = P_0 P^\| P_0[1 + (1 + \hat{g}(0)P_0 P^\| P_0)^{1/2}]^{-1}. \tag{6.13}$$

We note in passing that U is closely connected to a gauge transformation in Maxwell theory (cf [10]). We want to use the diagonal part of $\hat{H}_e(\boldsymbol{k})$, restricted to $(\mathcal{H}')^\perp$,

$$\hat{H}_e^{(0)}(\boldsymbol{k}) = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix}$$
$$= \begin{pmatrix} H_0(\boldsymbol{k}) + \|n\|_1 P^\perp P_0 P^\perp & 0 \\ 0 & P_0 \otimes \lambda^2 + Z_0 \otimes \{|\lambda s\rangle\langle\lambda^{-1}s| + |\lambda^{-1}s\rangle\langle\lambda s|\} + \|n\|_1 Z_0^2 \otimes |\lambda^{-1}s\rangle\langle\lambda^{-1}s| \end{pmatrix} \tag{6.14}$$

as the zero-order operator. A Fredholm argument, using the compactness of $[z^2 - H_0(\boldsymbol{k})]^{-1}$ on $(\mathcal{H}_1')^\perp$ implies that $H_1 = H_0(\boldsymbol{k}) + \|n\|_1 P^\perp P_0 P^\perp$, restricted to $(\mathcal{H}_1')^\perp$ has compact resolvent and discrete spectrum. On the other hand the operator

$$H_2 = P_0 \otimes \lambda^2 + Z_0 \otimes \{|\lambda s\rangle\langle\lambda^{-1}s| + |\lambda^{-1}s\rangle\langle\lambda s|\} + \|n\|_1 Z_0^2 \otimes |\lambda^{-1}s\rangle\langle\lambda^{-1}s| \tag{6.15}$$

acting in $\mathcal{H}_2'$, has a rather complicated structure due to the dependence on $Z_0 = Z_0(P_0 P^\| P_0)$. According to (A.21) it is non-negative definite and its restriction to $P_0 \mathcal{H}_1' \otimes L^2(\mathbb{R}, d\lambda)$ has empty null space, as is readily checked. Its spectrum is purely absolutely continuous and unitarily equivalent to that of $P_0 \otimes \lambda^2$ as we shall now discuss. Since $P_0 P^\| P_0$ is bounded, selfadjoint, it has the spectral decomposition $P_0 P^\| P_0 = \int \mu E\,(\mathrm{d}\mu)$, so

$$P_0 = \int E\,(\mathrm{d}\mu) \qquad Z_0 = \int \xi(\mu)E\,(\mathrm{d}\mu) \qquad \xi(\mu) = \mu[1 + (1 + \hat{g}(0)\mu)^{1/2}]^{-1} \tag{6.16}$$

and

$$H_2 = \int E\,(\mathrm{d}\mu) \otimes h(\mu) \tag{6.17}$$

with

$$h(\mu) = \lambda^2 + \xi(\mu)\{|\lambda s\rangle\langle\lambda^{-1}s| + |\lambda^{-1}s\rangle\langle\lambda s|\} + \|n\|_1 \xi(\mu)^2 |\lambda^{-1}s\rangle\langle\lambda^{-1}s|$$
$$= \lambda^2 + |u + v\rangle\langle u + v| - |v\rangle\langle v| = h_0 + |u + v\rangle\langle u + v| - |v\rangle\langle v| = h_0 + w \tag{6.18}$$

where $|u\rangle = \|n\|_1^{1/2}\xi(\mu)|\lambda^{-1}s\rangle$ and $|v\rangle = \|n\|_1^{-1/2}|\lambda s\rangle$. The perturbation w being finite rank, the absolutely continuous part of $h(\mu)$ is unitarily equivalent to that of λ^2, i.e. $[0, \infty)$. It is readily checked that 0 is not an eigenvalue of $h(\mu)$ and that there are no eigenvalues or resonances for $\mu = 0$ since then ξ vanishes and $h(\mu)$ reduces to λ^2. To treat the remaining cases we note that the resolvent $R(\zeta) = [\zeta - H]^{-1}$ of

$$H = H_0 + \alpha|a\rangle\langle a| + \beta|b\rangle\langle b| \tag{6.19}$$

can be given in terms of $R_0(\zeta) = [\zeta - H_0]^{-1}$ by Krein's formula,

$$R(\zeta) = R_0(\zeta) + R_0(\zeta)\Gamma(\zeta)^{-1}[\Gamma_b|a\rangle\langle a| + \Gamma_a|b\rangle\langle b| + \langle a|R_0(\zeta)|b\rangle|a\rangle\langle b|$$

$$+ \langle b|R_0(\zeta)|a\rangle|b\rangle\langle a|]R_0(\zeta)$$

$$\Gamma_a(\zeta) = \alpha^{-1} - \langle a|R_0(\zeta)|a\rangle \qquad \Gamma_b(\zeta) = \beta^{-1} - \langle b|R_0(\zeta)|b\rangle \tag{6.20}$$

$$\Gamma(\zeta) = \Gamma_a(\zeta)\Gamma_b(\zeta) - \langle a|R_0(\zeta)|b\rangle\langle b|R_0(\zeta)|a\rangle.$$

Applying this to the case at hand and setting $\zeta = z^2$ we find eventual eigenvalues or resonances z_j of H_2 as the zeros of $\Gamma(z^2)$. They have to satisfy

$$\hat{g}(z_j) = -\xi(\mu)^{-1}[2 + \xi(\mu)\hat{g}(0)]^{-1} \tag{6.21}$$

where the right-hand side is real, negative, so Im $\hat{g}(z_j)$ must vanish. Since z_j does not depend on μ, the right-hand side of (6.21) must be constant. This is only possible if μ takes on a single value. However, $E\,(\mathrm{d}\mu)$ is not concentrated in a single point μ. If this were true $P_0 P^\parallel P_0$ would be proportional to a projector, which is not the case for non-trivial P_0. Thus, generically, H_2 has no eigenvalues or resonances.

6.4. Applying the Fredholm theorem

We have

$$R(z^2) = [z^2 - \hat{H}_e(\boldsymbol{k})]^{-1} = z^{-2}P_e^\parallel + [z^2 - \hat{H}_e(\boldsymbol{k})^\perp]^{-1}P_e^\perp \tag{6.22}$$

where the projector upon the null space of $\hat{H}_e(\boldsymbol{k})$ and its complement are

$$P_e^\parallel = \begin{pmatrix} P^\parallel & 0 \\ 0 & 0 \end{pmatrix} \qquad P_e^\perp = \begin{pmatrix} P^\perp & 0 \\ 0 & 1 \end{pmatrix}. \tag{6.23}$$

Abbreviating $H = \hat{H}_e(\boldsymbol{k})^\perp = H^{(0)} + V$, $H^{(0)} = \hat{H}_e^{(0)}(\boldsymbol{k})^\perp = H_1 \oplus H_2$, $R(z^2) = [z^2 - H]^{-1}$, $R_0(z^2) = [z^2 - H^{(0)}]^{-1} = [z^2 - H_1]^{-1} \oplus [z^2 - H_2]^{-1} = R_1(z^2) \oplus R_2(z^2)$, we write

$$R(z^2) = R_0(z^2)[1 - VR_0(z^2)]^{-1} = R_0(z^2)[1 - K(z)]^{-1} = R_0(z^2)[1 + K(z)][1 - K(z)^2]^{-1}. \tag{6.24}$$

Since

$$K(z) = VR_0(z^2) = \begin{pmatrix} 0 & V_{12}R_2 \\ V_{21}R_1 & 0 \end{pmatrix} \tag{6.25}$$

we have

$$[K(z)^2]^*K(z)^2 = \begin{pmatrix} R_1^*V_{12}R_2^*V_{21}V_{12}R_2V_{21}R_1 & 0 \\ 0 & R_2^*V_{21}R_1^*V_{12}V_{21}\dot{R}_1V_{12}R_2 \end{pmatrix} \tag{6.26}$$

and its trace is

$$\mathrm{tr}[K(z)^2]^*K(z)^2 = \mathrm{tr}_1\{(V_{12}R_2V_{21})^*(V_{12}R_2V_{21})R_1R_1^* + R_1^*V_{12}V_{21}R_1V_{12}R_2R_2^*V_{21}\} \tag{6.27}$$

where tr_1 indicates a trace relative to $(\mathcal{H}_1')^\perp$. Here $R_1(z^2)$ is Hilbert–Schmidt, so it suffices to show that the remaining terms in the above expression are bounded operators. We encounter ($R_2^*R_2 = (\bar{z}^2 - z^2)^{-1}\{R_2 - R_2^*\}$ by the resolvent formula)

$$V_{12}V_{21} = P^\perp P_0\{\|s\|^4 Z_0(2 + \|\lambda^{-1}s\|^2 Z_0) + \|\lambda s\|^2\}P_0 P^\perp \tag{6.28}$$

and

$$\mathsf{V}_{12}\mathsf{R}_2\mathsf{V}_{21} = P^\perp P_0[\|s\|^4 Z_0^2 \langle \lambda^{-1}s|\mathsf{R}_2|\lambda^{-1}s\rangle + \|n\|_1 Z_0\{\langle \lambda^{-1}s|\mathsf{R}_2|\lambda s\rangle + \} + \langle \lambda s|\mathsf{R}_2|\lambda s\rangle]P_0 P^\perp.$$
(6.29)

The first is obviously bounded and this is also true for the second as follows from (6.14)–(6.20). The situation is not altered for the real and complex dilated cases, provided we remain in the appropriate analyticity domains. Thus

$$\mathsf{R}(z^2, \zeta) = \mathsf{R}_0(z^2, \zeta)[1 + \mathsf{K}(z, \zeta)][1 - \mathsf{K}(z, \zeta)^2]^{-1}$$
(6.30)

with $\mathsf{K}(z, \zeta)$ compact. Then the analytic Fredholm theorem tells us that, apart from the essential spectrum $\exp[-2\mathrm{i}\psi]\overline{\mathbb{R}}^+$ of $\mathsf{R}_0(z^2, \zeta)$, $\mathsf{R}(z^2, \zeta)$ can only have poles in the sector $\mathcal{S}(-2\psi) \cup \mathbb{R}^+$. Another result, obtained using an argument given in [16], tells us that for $\psi = 0$ the selfadjoint operator $\hat{\mathsf{H}}_e(\boldsymbol{k})^\perp$ has purely absolutely continuous spectrum $[0, \infty)$. Thus we have proven the following theorem.

Theorem 6.1. *Suppose that A_1–A_3 and A_5' hold. Then $\hat{\mathsf{H}}_e(\boldsymbol{k})$ has spectrum consisting of the infinitely degenerate eigenvalue zero and the absolutely continuous spectrum $[0, \infty)$. Moreover it has a dilatation-analytic continuation $\hat{\mathsf{H}}_e(\boldsymbol{k}, \zeta)$, $\zeta = \vartheta + \mathrm{i}\psi$, which has as essential spectrum the set (including the infinitely degenerate eigenvalue zero) $\sigma(\psi) = \exp[-2\mathrm{i}\psi]\overline{\mathbb{R}}^+$ and, possibly, real and complex eigenvalues of finite multiplicity in the sector $\mathcal{S}(-2\psi) \cup \mathbb{R}^+$.*

Corollary 6.2. *Under the same assumptions the statements of the theorem apply to $\mathsf{H}_e(\boldsymbol{k})$, in particular it has an analytic continuation $\mathsf{H}_e(\boldsymbol{k}, \zeta)$ with the same spectral properties as $\hat{\mathsf{H}}_e(\boldsymbol{k}, \zeta)$.*

Proof. Since $\hat{\mathsf{H}}_e(\boldsymbol{k})$ and $\mathsf{H}_e(\boldsymbol{k})$ are unitarily related, the statements for $\mathsf{H}_e(\boldsymbol{k})$ directly follow. Next we note that in

$$[z^2 - \mathsf{H}_e(\boldsymbol{k}, \vartheta)]^{-1} = U(\vartheta)[z^2 - \hat{\mathsf{H}}_e(\boldsymbol{k}, \vartheta)]^{-1}U^{-1}(\vartheta)$$

the continuation $\vartheta \to \zeta = \vartheta + \mathrm{i}\psi$ also affects $U(\vartheta)$ and $U^{-1}(\vartheta)$,

$$U(\vartheta) \to U(\zeta) \qquad U^{-1}(\vartheta) \to U^{-1}(\zeta).$$

However, as is seen from the Bloch-decomposed version of (A.12), these continuations exist as a bounded operator and are analytic in ζ, so $[z^2 - \mathsf{H}_e(\boldsymbol{k}, \vartheta)]^{-1}$ can be continued analytically

$$[z^2 - \mathsf{H}_e(\boldsymbol{k}, \vartheta)]^{-1} \to [z^2 - \mathsf{H}_e(\boldsymbol{k}, \zeta)]^{-1} = U(\zeta)[z^2 - \hat{\mathsf{H}}_e(\boldsymbol{k}, \zeta)]^{-1}U^{-1}(\zeta)$$

and the spectral statements directly follow. $\qquad\square$

In figure 1 we give a picture of the generic situation, bands in the lower half plane between the positive real axis and the essential spectrum, a half-line starting in zero and going off under an angle -2ψ. The bands emerge from the complex eigenvalues as $\boldsymbol{k}$ runs through the Brillouin zone.

7. A representation for $\mathsf{R}_e(z, \boldsymbol{k})$ and complex eigenvalues

In this section we discuss a representation for $\mathsf{R}_e(z, \boldsymbol{k})$ in terms of poles in the lower half plane, thus augmenting our earlier result (5.12). These poles are eigenvalues of the complex-dilated $\mathsf{H}_e(\boldsymbol{k}, \zeta)$ and we also consider the latter and the associated eigenvectors. Below we shall suppress $\boldsymbol{k}$ at various places and also $\boldsymbol{x}$ in $\varepsilon(\boldsymbol{x}, z)$ for brevity.
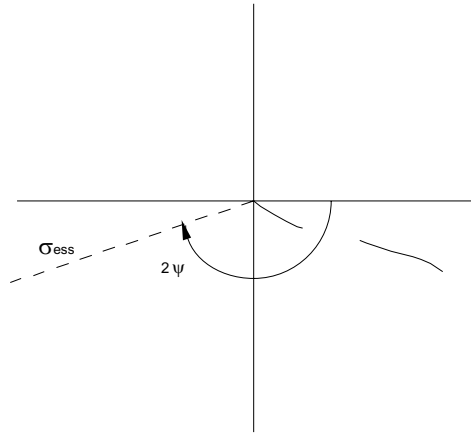
Figure 1. The complex dilated spectrum. The dashed curve is the rotated essential spectrum and the pieces in the fourth quadrant are the complex bands.

7.1. A representation for $R_e(z, \boldsymbol{k})$

We assume that A_1–A_3 and A_5' are satisfied. Then, for $\mathrm{Im}\, z > 0$,

$$R_e(z)P_1 = P_1[z^2 - H_e]^{-1}P_1 = P_1 U_d(\vartheta)[z^2 - H_e]^{-1}U_d(\vartheta)^{-1}P_1 = P_1[z^2 - H_e(\vartheta)]^{-1}P_1$$
$$= P_1[\xi - H_e(\zeta)]^{-1}P_1 = P_1 R(\xi, \zeta)P_1 = R_1(\xi, \zeta)P_1 \qquad (7.1)$$

where $\zeta = \vartheta + \mathrm{i}\psi$, $\psi \in [0, \beta]$ and $\xi = z^2$. Note that ξ runs through $\mathbb{C}\backslash\overline{\mathbb{R}}^+$ as z runs through $\mathbb{C}^+$. We can now continue $R(\xi, \zeta)$ in ξ across the positive real axis. In fact it is meromorphic in ξ on $\mathbb{C}\backslash\Gamma(-2\psi)$, $\Gamma(-2\psi)$ being the essential spectrum of $H_e(\zeta)$, with possible poles ξ_s in $\mathcal{S}(-2\psi) \cup \mathbb{R}^+$. Thus

$$R(\xi, \zeta) = \sum_{r \in \mathcal{A}(\psi)} [\xi - \xi_r]^{-1}P_r(\zeta) + R''(\xi, \zeta)$$
$$= \sum_{r,\alpha \in \mathcal{B}(\psi)} [\xi - \xi_r]^{-1}|\boldsymbol{v}_{r\alpha}(\zeta)\rangle\langle \boldsymbol{w}_{r\alpha}(\bar{\zeta})| + R''(\xi, \zeta) \qquad \xi \in \mathbb{C}\backslash\Gamma(-2\psi) \qquad (7.2)$$

where $R''(\xi, \zeta)$ is analytic in $\mathbb{C}\backslash\Gamma(-2\psi)$. We have the biorthogonality relation

$$\langle \boldsymbol{w}_{r\alpha}(\bar{\zeta})|\boldsymbol{v}_{r'\alpha'}(\zeta)\rangle = \delta_{rr'}\delta_{\alpha\alpha'}. \qquad (7.3)$$

Note that $R''(\xi, \zeta)$ and the sets $\mathcal{A}$ and $\mathcal{B}$ depend on ψ. Indeed, if the dilatation angle ψ is increased, more poles are uncovered. Note further that

$$|\boldsymbol{v}_{r\alpha}(\zeta)\rangle = \begin{pmatrix} |\boldsymbol{v}_{r\alpha 1}\rangle \\ |\boldsymbol{v}_{r\alpha 2}(\zeta)\rangle \end{pmatrix} \qquad (7.4)$$

where $|\boldsymbol{v}_{r\alpha 1}\rangle$ does not depend on ζ since the dilatation transformation only acts in $\mathcal{H}_2$. The same is true for $R_1(z, \zeta) = P_1 R(\xi, \zeta)P_1 = R_e(z, \zeta)P_1$, although the two terms on the right-hand side of

$$R_1(z) = P_1 R(\xi, \zeta)P_1 = \sum_{r,\alpha \in \mathcal{B}(\psi)} [\xi - \xi_r]^{-1}|\boldsymbol{v}_{r\alpha 1}\rangle\langle \boldsymbol{w}_{r\alpha 1}| + R_1''(\xi, \zeta) \qquad (7.5)$$

each depend on ψ. Since $[\xi - \xi_r]^{-1} = [z^2 - \xi_r]^{-1} = (2\sqrt{\xi_r})^{-1}\{[z - \sqrt{\xi_r}]^{-1} - [z + \sqrt{\xi_r}]^{-1}\}$, and setting $\lambda_r = -\sqrt{\xi_r}$

$$R_e(z) = \sum_{r,\alpha \in \mathcal{B}(\psi)} [z^2 - \xi_r]^{-1}|\boldsymbol{v}_{r\alpha 1}\rangle\langle \boldsymbol{w}_{r\alpha 1}| + R_e''(z^2, \zeta)$$

$$= \sum_{r,\alpha \in \mathcal{B}(\psi)} [z - \lambda_r]^{-1}(2\lambda_r^{-1}|v_{r\alpha 1}\rangle\langle w_{r\alpha 1}|)$$

$$+ \sum_{r,\alpha \in \mathcal{B}(\psi)} [z + \lambda_r]^{-1}(-2\lambda_r)^{-1}|v_{r\alpha 1}\rangle\langle w_{r\alpha 1}| + \mathsf{R}_e''(z^2, \zeta)$$

$$= \sum_{r,\alpha \in \mathcal{B}(\psi)} [z - \lambda_r]^{-1}(2\lambda_r)^{-1}|v_{r\alpha 1}\rangle\langle w_{r\alpha 1}| + \mathsf{R}_e'''(z, \zeta). \tag{7.6}$$

Comparing (7.6) and (5.12) we conclude that

$$\mathsf{A}_r = (2\lambda_r)^{-1}\sum_\alpha |v_{r\alpha 1}\rangle\langle w_{r\alpha 1}| \qquad r \neq 0 \tag{7.7}$$

so

$$\mathsf{R}_e(z) = z^{-1}\mathsf{A}_0 + \sum_{r,\alpha \in \mathcal{B}(\psi)} [z - \lambda_r]^{-1}(2\lambda_r)^{-1}|v_{r\alpha 1}\rangle\langle w_{r\alpha 1}| + \mathsf{R}_e'(z). \tag{7.8}$$

Note that $\mathsf{R}_e'(z, \mathbf{k})$ vanishes if we can continue through all of $\mathbb{C}^-$.

7.2. Eigenvalues and eigenvectors

Next we consider the eigenvalue problem

$$\mathsf{H}_e(\mathbf{k}, \zeta)v = \lambda_r^2 v \qquad \lambda_r^2 \in \mathcal{S}(-2\psi) \tag{7.9}$$

where $\text{Im}\,\zeta = -\psi < 0$ and λ_r in the previous section are given by $\lambda_r = -\sqrt{\lambda_r^2}$ and $v = v_{r\alpha}$. Here v has two components, $v_1(\mathbf{x}) \in \mathcal{H}_1'$ and $v_2(\mathbf{x}, \lambda) \in \mathcal{H}_2'$ and, in terms of these,

$$\begin{cases} \{\mathsf{H}_0(\mathbf{k}) + \|n\|_1 P_0\}v_1 + P_0\langle u(\bar{\zeta})|v_2 = \lambda_r^2 v_1 \\ P_0 v_1 \otimes |u(\zeta)\rangle + P_0\lambda^2 \exp[-2\zeta]v_2 = \lambda_r^2 v_2. \end{cases} \tag{7.10}$$

Hence

$$v_2 = P_0 v_2 = [\lambda_r^2 - \lambda^2 \exp[-2\zeta]]^{-1}P_0 v_1 \otimes |u(\zeta)\rangle \tag{7.11}$$

and substituting this into the first equation of (7.16), we obtain, using various definitions and the properties (3.6),

$$[\lambda_r^2\{1 + P_0\hat{g}(\lambda_r)\} + \mathsf{H}_0(\mathbf{k})]v_1 = [\lambda_r^2\varepsilon(\mathbf{x}, \lambda_r) + \mathsf{H}_0(\mathbf{k})]v_1 = 0 \tag{7.12}$$

which is once more the Helmholtz eigenvalue equation (1.17), but now for λ_r^2 which can be in the lower half plane and with $\hat{g}(\lambda_r)$ and $\varepsilon(\mathbf{x}, \lambda_r)$ the corresponding analytically continued quantities. In the same way we can obtain w_1 by considering the adjoint equation. It satisfies

$$[\overline{\lambda_r^2\varepsilon(\mathbf{x}, \lambda_r)} + \mathsf{H}_0(\mathbf{k})]w_1 = 0. \tag{7.13}$$

In fact, defining the conjugation operation C according to $Cf = \bar{f}$, we have $C\mathsf{H}_e(\mathbf{k}, \zeta)C = \mathsf{H}_e(\mathbf{k}, \bar{\zeta}) = \mathsf{H}_e(\mathbf{k}, \zeta)^*$, so $w = Cv$ if λ_r is non-degenerate. In the degenerate case we can still choose the eigenvectors at this eigenvalue in such a way that $w_{r\alpha} = Cv_{r\sigma}$. Using (7.10) and its counterpart for w and noting that $n(\lambda)$ is even in λ, the biorthogonality condition $\langle w_{ra}|v_{r'\alpha'}\rangle = \delta_{rr'}\delta_{\alpha\alpha'}\mathsf{U}$ then results in

$$\int_{\mathcal{C}_0} d\mathbf{x}\, \overline{v_{r\alpha\mathbf{1}}(\mathbf{x})}v_{r'\alpha'1}(\mathbf{x})\{1 + 2\Psi_{\mathcal{A}_0}(\mathbf{x})\exp[\mathrm{i}\psi]\int_{\Gamma(-\psi)} d\lambda\, \lambda^2[\lambda^2 - \lambda_r^2]^{-1}[\lambda^2 - \lambda_{r'}^2]^{-1}n(\lambda)\}$$

$$= \delta_{rr'}\delta_{\alpha\alpha'} \tag{7.14}$$

which fixes the normalization. It is instructive to consider the spatially homogeneous case. Here we can choose the unit cell at will. Once it is fixed, we obtain, since now $P_0 = 1$,

$$[\lambda_r^2\varepsilon(\lambda_r) + \mathsf{H}_0(\mathbf{k})]v_1 = 0 \tag{7.15}$$

where $\varepsilon(\lambda_r)$ only depends on λ_r. Generically $\lambda_r^2 \varepsilon(\lambda_r) \neq 0$, so v_1 is transverse and we have

$$[\lambda_r^2 \varepsilon(\lambda_r) + p^2(k)]v_1 = 0. \tag{7.16}$$

The solutions are determined by the boundary conditions as discussed in section 4. Thus

$$v_{nj1}(k) \sim e_j(k + k_n) \exp[i(k + k_n) \cdot x] \tag{7.17}$$

where the $e_j(k + k_n)$, $j = 1, 2$, are two orthogonal unit vectors, both orthogonal to $k + k_n$ and λ_r is determined by

$$\lambda_r^2 \varepsilon(\lambda_r) = (2\pi)^2(k + k_n)^2. \tag{7.18}$$

Since the functions $v_{nj1}(k)$ span $P^\perp \mathcal{H}_1'$, it follows directly that $\mathsf{R}_e'(z, k)$ reduces to $z^{-2} P^\parallel$.

8. Discussion

Our discussion of the properties of absorptive photonic crystals is based upon the knowledge of a single object, the electric susceptibility $\chi(x, t)$, or, equivalently, of $\hat{\chi}(x, z)$ or $\nu(x, \lambda)$. These quantities can be measured in bulk materials and this allows the theoretical prediction of the band structure of photonic crystals made up from such materials. However, so far mainly non-absorptive systems were considered and here we have made a first step towards a corresponding theoretical description of absorptive ones. In order to do so we made a few mathematical assumptions and below we shall briefly comment upon their physical origins. Then, without going into rigorously proving its existence (which can probably be justified using techniques developed for Schrödinger operators), we make a few comments about the local density of states. Finally we present some numerical results about the complex band structure for a simple absorbing one-dimensional model and give an outlook concerning future work.

8.1. The basic assumptions

The general linear relation between the polarization and field for an isotropic system is

$$P(x, t) = \int_{-\infty}^{+\infty} ds \int dy \, \chi(x, y, t - s)E(y, s) \tag{8.1}$$

which can be approximated at optical frequencies by

$$P(x, t) = \int_{-\infty}^{+\infty} ds \, \chi(x, t - s)E(x, s) \qquad \chi(x, t) = \int dy \chi(x, y, t). \tag{8.2}$$

This is justified by experimental observation and can also be understood by considering linear response expressions for χ, which show that it varies on a spatial scale of atomic dimensions, i.e. about a 1000 times smaller than an optical wavelength. Causality requires that the polarization at time t does not depend on the field at later times, thus reducing the upper value in the integral to t, i.e.

$$P(x, t) = \int_{-\infty}^{t} ds \, \chi(x, t - s)E(x, s). \tag{8.3}$$

A typical situation described by Maxwell's equations (1.1) is that of an electromagnetic wave passing through a piece of material. Initially an electromagnetic wavepacket is produced in a bounded space region away from the material and the fields and currents inside the latter vanish. Maxwell's equations being hyperbolic, it takes a non-zero time for the wave to reach

it. Then we can assume that at a finite time $t = t_0$ the material is reached and the polarization $\boldsymbol{P}$ starts to build up. Hence

$$\boldsymbol{P}(\boldsymbol{x}, t) = \int_{t_0}^{t} \mathrm{d}s \, \chi(\boldsymbol{x}, t - s) \boldsymbol{E}(\boldsymbol{x}, s) \qquad t \geqslant t_0. \tag{8.4}$$

Note that this simplification depends on the assumed initial situation and is not generally valid. It does not apply to a true photonic crystal since the spatial periodicity requires it to be infinite. However, actual measurements are done on finite systems, which are sufficiently large to make spectral information about the infinite system relevant for the case at hand.

We note in passing that a conservative system can emerge as a reasonable approximation in case $\chi(\boldsymbol{x}, t)$ is rapidly decaying in t. Then

$$\int_{t_0}^{t} \mathrm{d}s \, \chi(\boldsymbol{x}, t - s) \boldsymbol{E}(\boldsymbol{x}, s) = \int_{0}^{t - t_0} \mathrm{d}s \, \chi(\boldsymbol{x}, s) \boldsymbol{E}(\boldsymbol{x}, t - s)$$

$$\approx \int_{0}^{t - t_0} \mathrm{d}s \, \chi(\boldsymbol{x}, s) \boldsymbol{E}(\boldsymbol{x}, t) \approx \int_{0}^{\infty} \mathrm{d}s \, \chi(\boldsymbol{x}, s) \boldsymbol{E}(\boldsymbol{x}, t) \tag{8.5}$$

so

$$\boldsymbol{D}(\boldsymbol{x}, t) \approx \varepsilon_{\mathrm{stat}}(\boldsymbol{x}) \boldsymbol{E}(\boldsymbol{x}, t) \tag{8.6}$$

where $\varepsilon_{\mathrm{stat}}(\boldsymbol{x})$, the static permeability, is given by

$$\varepsilon_{\mathrm{stat}}(\boldsymbol{x}) = 1 + \chi_{\mathrm{stat}}(\boldsymbol{x}) \qquad \chi_{\mathrm{stat}}(\boldsymbol{x}) = \int_{0}^{\infty} \mathrm{d}s \, \chi(\boldsymbol{x}, s). \tag{8.7}$$

We obtain the current by differentiation,

$$\boldsymbol{J}(\boldsymbol{x}, t) = \partial_t \boldsymbol{P}(\boldsymbol{x}, t) = \chi(\boldsymbol{x}, 0) \boldsymbol{E}(\boldsymbol{x}, t) + \int_{t_0}^{t} \mathrm{d}s \, \partial_t \chi(\boldsymbol{x}, t - s) \boldsymbol{E}(\boldsymbol{x}, s) \qquad t \geqslant t_0. \tag{8.8}$$

Assuming that there is no abrupt current surge at $t = t_0$ this leads to the requirement $\chi(\boldsymbol{x}, 0) = 0$, which is part of assumption A_1. The assumed differentiability of $\chi(\boldsymbol{x}, t)$ is consistent with the idea that we are considering a macroscopic system, whereas its absolute integrability is based upon the observation that it is a rapidly decaying function of time for common dielectrics. The positivity of $\nu(\boldsymbol{x}, \lambda)$ in A_2 can be established experimentally but also microscopic linear response expressions lead to this property, provided the zero-order system, whose linear response to an electric field is studied, is passive, i.e. its density operator is a decreasing function of energy. Here we note that it is possible to create situations where $\nu(\boldsymbol{x}, \lambda)$ can be negative in certain λ-intervals by establishing a population inversion (for instance by exciting the states of atoms embedded in the material). Such 'systems with gain' [17] merit further investigation. One expects to find complex poles in both, the upper and lower half planes. Assumption A_3 is of a technical nature, it facilitates perturbation arguments. Without it one has to employ a form-perturbation technique, which is more complicated. Finally, assumptions A_4–A_6 are of a mathematical nature. Given the experimental accuracy it is always possible to obtain a satisfactory fit with functions satisfying such conditions. However, there are more restrictive theoretical models. An example is that of a spatially homogeneous gas of non-interacting two-level atoms with the atoms initially in their ground states. For this system the linear polarization, due to an external electric field, can be calculated [18], with the result ($\rho > 0$ is the gas density, κ and γ are positive constants)

$$\chi(\omega) = \kappa \rho ([\omega + \omega_0 + \mathrm{i}\gamma]^{-1} - [\omega - \omega_0 + \mathrm{i}\gamma]^{-1}) \tag{8.9}$$

leading to

$$\chi(t) = 2\kappa \rho \exp[-\gamma t] \sin \omega_0 t \qquad t \geqslant 0 \tag{8.10}$$

and

$$\hat{g}(z) = 2\kappa\rho\frac{z + \mathrm{i}\gamma}{(z + \mathrm{i}\gamma)^2 - \omega_0^2} \qquad n(\lambda) = 8\kappa\rho\frac{\gamma\omega_0\lambda^2}{[(\lambda - \omega_0)^2 + \gamma^2][(\lambda + \omega_0)^2 + \gamma^2]}. \qquad (8.11)$$

In this case A_3 is not satisfied and the analytic continuations in A_4 and A_5 are restricted due to the poles in $\pm\omega_0 - \mathrm{i}\gamma$. It may well be that such poles only cause harmless zeros in quantities such as $R_e(z)$ but this is certainly a topic for future research.

8.2. The local density of states

The density of states $N_\omega = \int \mathrm{d}x\, N_\omega(x)$ for conservative systems can be defined through an eigenvalue counting procedure, leading to the expression

$$N_\omega(x) = \mathrm{Im}\ \mathrm{tr}\langle x|[(\omega + \mathrm{i}0)^2\varepsilon(x) - \mathsf{H}_0]^{-1}|x\rangle$$
$$= \int_{\mathcal{B}} \mathrm{d}k\, \mathrm{Im}\ \mathrm{tr}\langle x|[(\omega + \mathrm{i}0)^2\varepsilon(x) - \mathsf{H}_0(k)]^{-1}|x\rangle \qquad x \in \mathcal{C}_0 \qquad (8.12)$$

for $N_\omega(x)$, the local density of states. Here the trace tr is over a 3×3 matrix (note that $\mathsf{H}_0(k)$ is an operator-valued 3×3 matrix). The latter appears as a factor in the spontaneous radiative decay rate $\Gamma(x)$ of an atom embedded in a dielectric in the position x. Γ can be obtained from Fermi's golden rule or a similar procedure [19]. In absorptive situations N_ω is no longer defined in terms of counting eigenvalues, the latter becoming complex. However, (8.10) still appears in Γ, but with $\varepsilon(x)$ replaced by $\varepsilon(x, \omega + \mathrm{i}0)$, cf [10]. According to (7.8) we then have

$$N_\omega(x) = \mathrm{Im}\ \sum_{r,\alpha} \int_{\mathcal{B}} \mathrm{d}k\, [\omega + \mathrm{i}0 - \lambda_r(k)]^{-1}(2\lambda_r)^{-1}\langle x|v_{r\alpha 1}(k)\rangle \cdot \langle w_{r\alpha 1}(k)|x\rangle$$
$$+ \mathrm{Im}\ \mathrm{tr}\langle x|R'_e(k, \omega + \mathrm{i}0)|x\rangle$$
$$= \mathrm{Im}\ \sum_{r,\alpha} \int_{\mathcal{B}} \mathrm{d}k\, [\omega + \mathrm{i}0 - \lambda_r(k)]^{-1}(2\lambda_r)^{-1}|\langle x|v_{r\alpha 1}(k)\rangle|^2$$
$$+ \mathrm{Im}\ \mathrm{tr}\langle x|R'_e(k, \omega + \mathrm{i}0)|x\rangle \qquad (8.13)$$

where $\omega + \mathrm{i}0$ can be replaced by ω if $\lambda_r(k)$ has a non-zero imaginary part. We also used the fact that $\langle w_{r\alpha 1}(k)|x\rangle = \overline{\langle x|v_{r\alpha 1}(k)\rangle}$. In general there can be contributions of other type in the second term. As we have seen there are no real poles outside 0 if $n(\lambda)$ is non-vanishing on $\mathbb{R}$ and the second term is absent if we can continue throughout $\mathbb{C}^-$. Then N_ω is in general non-vanishing for any ω. In the conservative case R'_e is absent and in the present situation it may also contain only pole contributions although our approach does not allow us to draw this conclusion.

8.3. An absorbing one-dimensional model

We calculated the low-frequency band structure for a simple periodic, layered, medium with interfaces parallel to the YZ-plane with piecewise constant ε, independent of the y and z coordinates, i.e.,

$$\varepsilon(x) = \begin{cases} \varepsilon_s & x \in (na - \frac{r_s}{2}, na + \frac{r_s}{2}) \\ \varepsilon_b & x \notin (na - \frac{r_s}{2}, na + \frac{r_s}{2}) \end{cases} \qquad (8.14)$$

where s stands for scatterer, b for background, $n \in \mathbb{Z}$, a is the lattice constant (length of the unit cell) and $0 < r_s < a/2$. We assume that ε_b is real, whereas ε_s is taken to be frequency
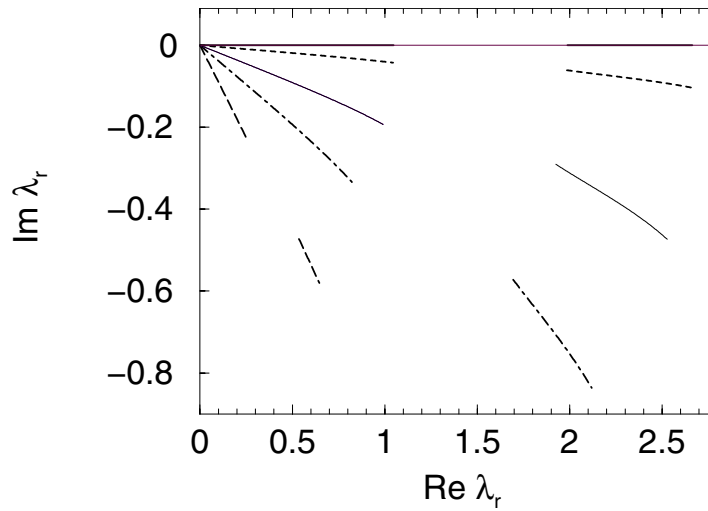
Figure 2. The lowest bands for a one-dimensional model for increasing values of Im ε. Here $\varepsilon_b = 1$, Re $\varepsilon_s = 12$ and Im $\varepsilon_s = 0$ (solid curves), 1, 5, 12 and 120.

independent but it may have a positive imaginary part. In the absence of field modes parallel to the interfaces the Helmholtz equation (7.12) for the normal field modes reduces to

$$[\lambda_r(k)^2 \varepsilon(x) - p^2(k)]\psi(x) = 0 \tag{8.15}$$

where $p^2(k)$ is $-\partial_x^2$ with the appropriate boundary condition, depending on k from the first Brillouin zone. In this case the analytic continuation of ε is trivial but nevertheless complex eigenvalues $\lambda_r(k)$ are found in the lower half plane. In figure 2 the resulting first few bands are displayed for $\varepsilon_b = 1$, Re $\varepsilon_s = 12$ and Im $\varepsilon_s = 0, 1, 5, 12$ and 120 for a filling fraction of the scatterers of 40%. In the long wavelength limit, $k \ll 1$, $\varepsilon(x)$ can be replaced by its average $\varepsilon_{\text{eff}} = \int_{\mathcal{C}_0} dx \, \varepsilon(x)$ and (8.15) reduces to $\lambda_r(k)^2 \varepsilon_{\text{eff}} = k^2$, giving the slope of the first complex band in terms of arg ε_{eff}. For further details, see [9].

8.4. Outlook

In view of the present results the next step is the calculation of actual band structures, in particular for lattices consisting of metallic particles, so that a comparison with existing calculations [6], where absorption is neglected, can be made. In addition the local density of states is being investigated, since, although band gaps may be absent, this quantity may well be small in regions where a gap would be present if absorption is neglected. Such work is now in progress for two- and three-dimensional systems. Another matter that has our attention, is the construction of a perturbation theory for the case of small absorption. Finally we note that in actual experimental situations finite systems are studied and absorption will set a limit to their size. Thus it is important to obtain an expression for the absorption per unit length for a fixed frequency and direction of propagation in order to obtain an estimate about the allowed size of a crystal. If the number of allowed unit cells becomes small, the present model of an infinite crystal is no longer acceptable and calculations should be done for finite systems.

Acknowledgments

Appendix. The null space of H_e and a unitary transformation

In establishing compactness properties the circumstance that H_e has an infinite-dimensional null space, $\mathcal{N} = \mathcal{N}(H_e)$, that does not coincide with the null space $\mathcal{N}_0 = \mathcal{N}(H_e^{(0)})$ of $H_e^{(0)}$ complicates matters significantly. It therefore makes sense to find a unitary transformation between the two and below we show how this is done. For brevity we suppress explicit x-dependencies and denote

$$H_e = \begin{pmatrix} H_0 + \|\sigma\|^2 & \langle \lambda\sigma| \\ |\lambda\sigma\rangle & \lambda^2 \end{pmatrix} \tag{A.1}$$

where $\|\sigma\|^2 = \int d\lambda\, \sigma(x,\lambda)^2$. As we have seen $f \in \mathcal{N}$ satisfies $H_0 f_1 = 0$ and $f_2 = -\lambda^{-1}\sigma(\lambda) f_1$, so $f_1 = P^\| f_1$ and $f_2 = -\lambda^{-1}\sigma(\lambda) P^\| f_1$ and we can represent f as

$$f = \begin{pmatrix} P^\| & 0 \\ -\lambda^{-1}\sigma(\lambda) P^\| & 0 \end{pmatrix} h = \begin{pmatrix} P^\| & 0 \\ -|\lambda^{-1}\sigma\rangle P^\| & 0 \end{pmatrix} = Ah \qquad h \in \mathcal{H}. \tag{A.2}$$

Then, using $\langle \lambda^{-1}\sigma | \lambda^{-1}\sigma\rangle = \hat{\chi}(0)$ and $1 + \hat{\chi}(0) = \varepsilon_{\text{stat}}$,

$$A^* = \begin{pmatrix} P^\| & -P^\|\langle\lambda^{-1}\sigma| \\ 0 & 0 \end{pmatrix} \qquad A^*A = \begin{pmatrix} P^\|\varepsilon_{\text{stat}} P^\| & 0 \\ 0 & 0 \end{pmatrix} \tag{A.3}$$

and $P_e^\|$, the projector upon $\mathcal{N}$, is given by

$$P_e^\| = A[A^*A]^{-1}A^* = \begin{pmatrix} X & -X\langle\lambda^{-1}\sigma| \\ -|\lambda^{-1}\sigma\rangle X & |\lambda^{-1}\sigma\rangle X \langle\lambda^{-1}\sigma| \end{pmatrix} \tag{A.4}$$

where $X = P^\|[P^\|\varepsilon_{\text{stat}} P^\|]^{-1} P^\|$. Its counterpart on $\mathcal{H}'$ after the Bloch decomposition has been made is obtained by replacing $|\lambda^{-1}\sigma\rangle$ by $P_0|\lambda^{-1}s\rangle$, etc. The unitary transformation that maps $\mathcal{N}_0$ onto $\mathcal{N}$ is

$$U^\| = A[A^*A]^{-1/2} P_0^\| = A X^{1/2} P_0^\| \qquad P_0^\| = \begin{pmatrix} P^\| & 0 \\ 0 & 0 \end{pmatrix}. \tag{A.5}$$

We now turn to $P_e^\perp = 1 - P_e^\|$, the projector upon the orthoplement $\mathcal{N}^\perp$ of $\mathcal{N}$. For $f \perp \mathcal{N}$ we must have $(f, Ag) = 0$, $\forall g \in \mathcal{H}$, so $A^* f = 0$, implying that $P^\| f_1 = P^\|\langle\lambda^{-1}\sigma | f_2$. Thus f is of the general form

$$f = \begin{pmatrix} P^\perp & P^\|\langle\lambda^{-1}\sigma| \\ 0 & 1 \end{pmatrix} g = Bg \qquad g \in \mathcal{H}. \tag{A.6}$$

Then

$$B^* = \begin{pmatrix} P^\perp & 0 \\ |\lambda^{-1}\sigma\rangle P^\| & 1 \end{pmatrix} \qquad B^*B = \begin{pmatrix} P^\perp & 0 \\ 0 & 1 + |\lambda^{-1}\sigma\rangle P^\|\langle\lambda^{-1}\sigma| \end{pmatrix} \tag{A.7}$$

and, since

$$[1 + |\lambda^{-1}\sigma\rangle P^\|\langle\lambda^{-1}\sigma|]^{-p} = 1 + |\lambda^{-1}\sigma\rangle P^\|[P^\|\langle\lambda^{-1}\sigma|\lambda^{-1}\sigma\rangle P^\|]^{-1}$$
$$\times \{[1 + P^\|\langle\lambda^{-1}\sigma|\lambda^{-1}\sigma\rangle P^\|]^{-p} - 1\} P^\|\langle\lambda^{-1}\sigma|$$

$$= 1 + |\lambda^{-1}\sigma\rangle P^{\parallel}[P^{\parallel}\hat{\chi}(0)P^{\parallel}]^{-1}P^{\parallel}\{[1 + P^{\parallel}\hat{\chi}(0)P^{\parallel}]^{-p} - 1\}P^{\parallel}\langle\lambda^{-1}\sigma|$$
$$= 1 + |\lambda^{-1}\sigma\rangle P^{\parallel}[P^{\parallel}\hat{\chi}(0)P^{\parallel}]^{-1}P^{\parallel}\{[P^{\parallel}\varepsilon_{\text{stat}}P^{\parallel}]^{-p} - 1\}P^{\parallel}\langle\lambda^{-1}\sigma|$$
$$= 1 + |\lambda^{-1}\sigma\rangle P^{\parallel}[P^{\parallel}\hat{\chi}(0)P^{\parallel}]^{-1}P^{\parallel}[X^p - 1]P^{\parallel}$$
$$\times \langle\lambda^{-1}\sigma| = 1 + |\lambda^{-1}\sigma\rangle Y_p\langle\lambda^{-1}\sigma|$$

we have

$$[B^*B]^{-p} = \begin{pmatrix} P^{\perp} & 0 \\ 0 & 1 + |\lambda^{-1}\sigma\rangle Y_p\langle\lambda^{-1}\sigma| \end{pmatrix} \tag{A.8}$$

where

$$Y_1 = -P^{\parallel}XP^{\parallel} \qquad Y_{1/2} = -P^{\parallel}X[1 + X^{1/2}]^{-1}P^{\parallel}. \tag{A.9}$$

Thus

$$P_e^{\perp} = B[B^*B]^{-1}B^* = \begin{pmatrix} P^{\perp} + P^{\parallel}\hat{\chi}(0)P^{\parallel}X & X\langle\lambda^{-1}\sigma| \\ |\lambda^{-1}\sigma\rangle X & 1 - |\lambda^{-1}\sigma\rangle X\langle\lambda^{-1}\sigma| \end{pmatrix} \tag{A.10}$$

and it is easily verified that indeed $P_e^{\parallel} + P_e^{\perp} = 1$. The unitary transformation $U^{\perp}$ that maps $\mathcal{N}_0^{\perp} = P_0^{\perp}\mathcal{H}$ onto $\mathcal{N}^{\perp}$ is given by

$$U^{\perp} = B[B^*B]^{-1/2}P_0^{\perp} = \begin{pmatrix} P^{\perp} & P^{\parallel}X^{1/2}P^{\parallel}\langle\lambda^{-1}\sigma| \\ 0 & 1 - |\lambda^{-1}\sigma\rangle P^{\parallel}X[1 + X^{1/2}]^{-1}P^{\parallel}\langle\lambda^{-1}\sigma| \end{pmatrix} \tag{A.11}$$

and the full unitary transformation is

$$U = U^{\parallel} \oplus U^{\perp} = \begin{pmatrix} P^{\perp} + P^{\parallel}X^{1/2}P^{\parallel} & P^{\parallel}X^{1/2}P^{\parallel}\langle\lambda^{-1}\sigma| \\ -|\lambda^{-1}\sigma\rangle P^{\parallel}X^{1/2}P^{\parallel} & 1 - |\lambda^{-1}\sigma\rangle P^{\parallel}X[1 + X^{1/2}]^{-1}P^{\parallel}\langle\lambda^{-1}\sigma| \end{pmatrix}. \tag{A.12}$$

Since U maps the null space of H_e onto that of $\mathsf{H}_e^{(0)}$, $U^* = U^{-1}$ does the reverse and it follows that $\mathsf{H}_e^{(0)}$ and

$$\hat{\mathsf{H}}_e = U^{-1}\mathsf{H}_eU \tag{A.13}$$

have the same null space. A straightforward calculation results in

$$\hat{\mathsf{H}}_e = \begin{pmatrix} \mathsf{H}_0 + P^{\perp}\|\sigma\|^2P^{\perp} & P^{\perp}\{\|\sigma\|^2Z\langle\lambda^{-1}\sigma| + \langle\lambda\sigma|\} \\ \{|\lambda^{-1}\sigma\rangle Z\|\sigma\|^2 + |\lambda\sigma\rangle\}P^{\perp} & \lambda^2 + |\lambda\sigma\rangle Z\langle\lambda^{-1}\sigma| + |\lambda^{-1}\sigma\rangle Z\langle\lambda\sigma| + |\lambda^{-1}\sigma\rangle Z\|\sigma\|^2Z\langle\lambda^{-1}\sigma| \end{pmatrix} \tag{A.14}$$

where

$$Z = P^{\parallel}X^{1/2}[1 + X^{1/2}]^{-1}P^{\parallel} = P^{\parallel}[1 + (P^{\parallel}\varepsilon_{\text{stat}}P^{\parallel})^{1/2}]^{-1}P^{\parallel}. \tag{A.15}$$

The corresponding expression for $\hat{\mathsf{H}}_e(\boldsymbol{k})$ is

$$\hat{\mathsf{H}}_e(\boldsymbol{k}) = \begin{pmatrix} \mathsf{H}_0(\boldsymbol{k}) + \|n\|_1P^{\perp}P_0P^{\perp} & P^{\perp}P_0\{\|n\|_1Z_0\langle\lambda^{-1}s| + \langle\lambda s|\} \\ \{\|n\|_1Z_0|\lambda^{-1}s\rangle + |\lambda s\rangle\}P_0P^{\perp} & P_0 \otimes \lambda^2 + Z_0 \otimes \{|\lambda s\rangle\langle\lambda^{-1}s| + |\lambda^{-1}s\rangle\langle\lambda s|\} + \|n\|_1Z_0^2 \otimes |\lambda^{-1}s\rangle\langle\lambda^{-1}s| \end{pmatrix} \tag{A.16}$$

where

$$Z_0 = P_0ZP_0 = P_0P^{\parallel}P_0[1 + (1 + \hat{g}(0)P_0P^{\parallel}P_0)^{1/2}]^{-1}. \tag{A.17}$$

A more precise expression for $\hat{\mathsf{H}}_e(\boldsymbol{k})_{22}$ is (I_1 is the unit operator on $\mathcal{H}_1'$)

$$\hat{\mathsf{H}}_e(\boldsymbol{k})_{22} = \mathsf{I}_1 \otimes \lambda^2 + Z_0 \otimes \{|\lambda s\rangle\langle\lambda^{-1}s| + |\lambda^{-1}s\rangle\langle\lambda s|\} \tag{A.18}$$

Note that we can rewrite this as

$$\hat{\mathsf{H}}_e(\boldsymbol{k})_{22} = \lambda\{1 - P_0\|s\|^{-2}|s\rangle\langle s|\}\lambda + \|s\|^{-2}\{Z_0\|n\|_1|\lambda^{-1}s\rangle + |\lambda s\rangle\}\{Z_0\|n\|_1\langle\lambda^{-1}s| + \langle\lambda s|\} \tag{A.19}$$

so, with

$$|u\rangle = Z_0\|n\|_1|\lambda^{-1}s\rangle + |\lambda s\rangle \tag{A.20}$$

we have

$$\hat{\mathsf{H}}_e(\boldsymbol{k}) = \begin{pmatrix} \mathsf{H}_0(\boldsymbol{k}) + \|n\|_1P^{\perp}P_0P^{\perp} & P^{\perp}P_0\langle u| \\ |u\rangle P_0P^{\perp} & \lambda\{1 - P_0\|n\|_1^{-1}|s\rangle\langle s|\}\lambda + \|n\|_1^{-1}|u\rangle\langle u| \end{pmatrix}. \tag{A.21}$$

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