VARIATIONAL CHARACTERIZATION OF RESONANT STATES IN SOME INTEGRATED OPTICAL DEVICES

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Abstract Two examples from integrated optics are described that motivate the use of explicit variational characterizations for physical parameters that are relevant for the functioning of optical devices. For 1D optical gratings the boundary of the bandgaps, and for 2D square micro-resonators the resonant frequency, are formulated as eigenvalues of the governing Helmholtz equation. This requires to define the set on which the corresponding functional is optimised in an appropriate way, depending on the application.

1. Introduction

In modern optical telecommunication, all-optical devices are used to manipulate light for various purposes. These (nano- and micro-meter scale) devices exploit interference properties to manipulate the light that is transported to and from the device through waveguides. For instance, a grating acts like a physical mirror for an interval of wavelengths in the so called 'band gap', while a filter will select a specific wavelength from a broad spectrum of light. For the design and actual fabrication of such devices it is desirable to have direct characterizations for the critical parameters, such as the boundaries of the band gap and the filtered wavelength. Dependence of these critical values on material properties and geometric dimensions are desired as well.

We will show in this paper that variational formulations can lead to extremal characterizations of such critical values. The variational approach has
another advantage that it is well suited for numerical discretizations, for instance it will lead in a standard way to consistent Finite Element procedures.

A major technical complication that has to be overcome is that such problems are typically modelled on unbounded domains. Although the device (and surrounding region where the changes in light are most essential) may be small, the presence of waveguides and the unavoidable radiation in unknown directions makes it difficult to 'confine' the problem, while this is desirable for mathematical analysis and numerical calculations.

We will consider in more detail the two examples of integrated optical devices mentioned above. The first device is a photonic crystal ([7]), a spatially periodic structure which can be impermeable for light in a certain range of wavelengths, the so called 'band-gap'. For the simplest case of a 1D crystal, then usually called 'grating', we will show that explicit variational methods can be used to characterize the boundaries of the bandgap. The second device is a so-called 'square micro-resonator' (see [1, 9, 10]), a square of high index material that can support various modes which may form a standing wave and let the square act like a cavity. Then a series of two squares can reroute light of one specific wavelength from one waveguide to another parallel waveguide, while other wavelengths remain practically unaffected. We will show that the wavelength of the rerouted light correspond to an eigenvalue of an eigenvalue problem, with Dirichlet conditions at a suitably rescaled square replacing the material interface conditions.

Both examples are planar structures, and we will assume the materials to be lossless (non-dissipative), nonmagnetic and linear. Then Maxwell's equations reduce for monochromatic light to inhomogeneous Helmholtz equations, which uncouple into a set of two scalar equations for two polarizations. Restricting to TE-polarization, a scalar equation results for the spatially dependent part of the perpendicular component of the electromagnetic field. Writing \( \mathbf{E}(x, z; t) = \mathbf{u}(x, z)e^{i\omega t} + \mathbf{c} \) the equation for the (complex valued) spatial dependence is the Helmholtz equation

\[
\left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + \frac{\omega^2}{c^2} n^2(x, z) \right] \mathbf{u} = 0, \quad (1.1)
\]

where \( \omega \) is the frequency of the light, related to the (vacuum-) wavelength \( \lambda \) according to \( \omega = \frac{2\pi}{\lambda} c \) with \( c \) the speed of light; \( n(x, z) \) denotes the index of refraction. Different materials correspond to different values of the index of refraction, and the space-dependency of the index defines implicitly the optical device. The weak form of Helmholtz' equation is understood: at the interface, continuity of the field and its normal derivative have to be imposed. When using the variational formulation of Helmholtz' equation, the interface
conditions arise as a natural consequence. Conditions at ‘infinity’ depend on
the type of applications one is interested in.

2. Characterization of band gaps in gratings

The first example is a 1D gratings. The index of refraction depends on
only one variable, \( z \), and changes periodically, say with period \( p \):

\[
\left[ \partial_z^2 + \frac{\omega^2}{c^2} n^2(z) \right] u = 0, \quad (2.1)
\]

\[ n(z + p) = n(z). \]

Often the case is considered that the index is piecewise constant. Such a gra-
ting is obtained for instance by positioning two materials of different constant
index in a periodic way behind each other. Light will be partially reflected
and partly transmitted at each interface, leading to summation of infinitely
many contributions at each position. In these cases the transfer matrix of one
period, and therefore the total solution of an infinite grating, can be written
down explicitly and all bandgaps can be found, although the relevant equa-
tions are transcendental. Here a ‘bandgap’ is an interval of frequencies for
which there is no light propagation through the structure. The method to be
described below is more generally applicable, for any periodic index variation,
and allows direct extension to nonlinear materials.

A first observation is that as a result of Floquet’s theorem, or Bloch’s
theorem, it follows that any solution can be written like

\[
u(z) = v(z, \omega) e^{ik(\omega)z}, \quad (2.2)
\]

where \( v(z, \omega) \) is a \( p \)-periodic function and the ‘wave number’ \( k(\omega) \) can be real
or complex. The intervals of values \( \omega \) for which \( k(\omega) \) is not real determine
the band-gaps, since then no finite-amplitude solutions exist and no light
propagation through the grating is possible. We will now characterize the
boundaries of the band gaps.

The essential idea is that the ‘boundary states’, i.e., the states that cor-
respond to the boundary of the band gap, satisfy the original equation (2.1)
together with some (skew-) symmetry condition that will be detailed further
on. Referring to (2.1), the variational principle

\[
\delta \int \left[ \left( \partial_z u \right)^2 - \frac{\omega^2}{c^2} n^2(z) u^2 \right] dz = 0
\]

leads to the correct equation, but is useless for the present purpose, since the
value of \( \omega \) is unknown and should be sought: our aim is to solve the eigenvalue
problem which includes the determination of the 'eigenvalue' \( \frac{\omega^2}{c^2} \), i.e., we have to deal with a free-frequency problem.

By multiplying the equation by the boundary state, say \( U \), an integration over the periodic interval, anticipating that boundary terms from partial integration will vanish, leads to the result

\[
 \frac{\omega^2}{c^2} = \int (\partial_z U)^2 dz \int [n^2(z) U^2] dz.
\]

This shows that the boundary value \( \omega \) is expressed as the value of a Rayleigh quotient evaluated at the boundary state \( U \).

Standard methods for linear eigenvalue problems deal with this problem by looking at the critical points of this Rayleigh quotient. In [2] constrained formulations are used since these can be generalized to nonlinear problems. One such formulation is

\[
 \frac{\omega^2}{c^2} = \text{crit} \left\{ \int (\partial_z u)^2 dz \left\| \int [n^2(z) u^2] dz = 1, \ u \in \mathcal{U} \right\} \right. \]

The set of competing functions in looking for a critical value is specified by the set \( \mathcal{U} \), which includes specification of the boundary or periodicity conditions on the specific interval. A critical point will satisfy, according to Langrange's multiplier rule, the correct equation with \( \frac{\omega^2}{c^2} \) as the Lagrange multiplier.

In the following we will restrict to the simplest case, the lowest band gap with \( Re(k) = \pi/p \), which we will denote by \( BG \) for simplicity, with lower and upper value given by

\[
 BG = [\Omega_-, \Omega_+].
\]

Since \( Re(k) = \pi/p \), it can be shown that the boundary states are actually \( 2p \) periodic and shift-skew-symmetric. Denoting the boundary state by \( w \), it holds

\[
 \partial_z^2 w + \frac{\omega^2}{c^2} n^2 w = 0, \ \text{for} \ \omega = \Omega_\pm
\]

and \( w(z + p) = -w(z) \).

Hence each solution is a shifted skew continuation of a solution in one period with Dirichlet boundary conditions. This can be translated to conditions of the solution on an interval of length \( p \). Namely, to retain smoothness in the odd continuation, except the vanishing boundary condition, the derivative at begin point, say \( \xi \), and endpoint, then \( \xi + p \), should be equal but of opposite sign:

\[
 w(\xi) = w(\xi + p) = 0; \ \partial_z w(\xi) = -\partial_z w(\xi + p).
\]

Since, in general, the precise position of the interval is unknown, we also have to find the position of the interval, i.e., the value of \( \xi \). That will be done in
the following, for which it is convenient to define the set that satisfy already
the Dirichlet conditions:

\[ \mathcal{W}_\xi^D = \{ w : [\xi, \xi + p] \to IR, w(\xi) = w(\xi + p) = 0 \}. \]

With only these Dirichlet conditions, one can define the eigenvalue problem,
and look for the lowest eigenvalue, that will depend on the choice of \( \xi \), say

\[ \frac{\Omega(\xi)^2}{c^2} = \frac{\Omega(\xi)}{c} \left\{ \int_{\xi}^{\xi + p} \left[ (\partial_z u)^2 \right] dz \right\} \left\{ \int_{\xi}^{\xi + p} \left[ n^2(z) u^2 \right] dz = 1, u \in \mathcal{W}_\xi^D \right\}. \]

With \( \Omega(\xi) \) defined in this way, the results can be summarized as follows. The
boundaries of the first (lowest) bandgap \( BG = [\Omega_-, \Omega_+] \) are given by the
extrema of the function \( \Omega(\xi) \):

\[ \Omega_- = \min_{\xi} \Omega(\xi), \quad \Omega_+ = \max_{\eta} \Omega(\xi). \]

It can be observed that the boundary-state corresponding to the lowest value
will have its maximal intensity at the high-index region and is found from a
constrained minimization problem. The boundary state corresponding to \( \Omega_+ \)
is found from a Max-Min problem, and is a saddle point of the constrained
formulation.

The proof is given in [2]; the essential ingredient is that the variation of the
position \( \xi \) of the interval produces the correct boundary condition for smooth
continuation, i.e., produces the remaining condition \( \partial_z w(\xi) = -\partial_z w(\xi + p) \)
at the extremal values for \( \xi \).

A few remarks may be appropriate. First, the above variational character-
izations are constructive in the sense that they can be used to develop
numerical programs: for fixed \( \xi \) the function space \( \mathcal{W}_\xi^D \) can be discretized,
after which the functionals can be reduced to finite dimensional functions;
the resulting finite dimensional extremal problem can then be solved and the
extreme values for \( \xi \) can be found (see [2]). Furthermore, higher band
will correspond to saddle points of the critical point problem. The character-
ization given here can be extended to non-linear materials with Kerr
nonlinearity by using the functional

\[ \int_{\xi}^{\xi + p} \left[ n^2(z) u^2 + \frac{1}{2} c u^4 \right] dz \]

instead of \( \int_{\xi}^{\xi + p} [n^2(z) u^2] dz \). The value of the constraint should then be
taken into account and the resulting bandgap boundaries, and boundary
states, will depend on the value of this constraint.
3. Resonant state of a square resonator

The second example is a 2D device that functions as a filter by selecting and rerouting light of one specific wave length. Disk- or ring-resonators, positioned between two parallel wave guides, are often used to that aim. Then light, caught by the resonator, travels around the circumference (in so-called whispering gallery modes) and interacts with the light of the incoming wave guide. When the interference is destructive, practically all light will continue its path through the wave guide. When the interference is constructive, light intensity will increase in the resonator and is then transmitted to the opposite wave guide. Complete constructive interference will take place for only one (or a discrete set of) wave length, explaining the filter property; see e.g. [1, 10, 11].

Instead of being based on travelling waves, a square resonator may exhibit the same phenomenon, but now with standing waves instead of travelling waves inside the resonator; see [5, 9, 4]. We will characterize one such resonant state in the following.

The geometric lay-out and phenomenon of a single square resonator is shown in the figure 1. The geometry is shown in the left of the fig (1a): light input through the lower wave guide(port A) interacts (through the evanescent field) with the square material. For specific wave lengths, internal modes are excited and form a field intensity as shown in the right picture of fig (1a). In this state, light is radiated in all four directions at (almost) equal amounts, as shown in the fig (1b).

![Figure : (1a)]
It is remarked that geometric dimensions should be chosen carefully since transfer properties depend sensitively on the geometry. Furthermore, practically speaking, the transfer is only sufficient if the index contrasts are sufficiently high; for more realistic material values, a modified device has been described in [6]. This modification places the cavity in between horizontal gratings, where the grating is designed such that it acts like a mirror, i.e. has its bandgap, in the relevant wavelength interval for the states of the cavity.

When two square resonators between two parallel waveguides are put in series, the effects of the squares superimpose and the configuration can act as a filter: specific wave lengths are transmitted from the lower-input port A to the upper-output port C, as shown in the figure (2a). The resonant field pattern is shown at the figure (2b).
The field patterns shown above, and the value of the corresponding resonant wavelength, have been found with pseudo-analytical methods, using mode expansion techniques with sets of 1D-modes in transversely uniform domains (see [8]). Then the resonant wavelengths and states are found after calculating a whole interval of wavelengths. Since the interest is mainly in the resonant case, a more direct approach is desired, and a variational formulation like an eigenvalue problem on the square seems very appealing. That is to say, one would like to find the resonant frequency, say $\Omega$, from a formulation like

$$\Omega^2 = \text{"crit" } \left\{ \int_S (\partial_x u + \partial_y u)^2 \right\} \left/ \int_S [n_S^2 u^2] \right. = 1, \quad u \in \mathcal{U}_S \right\}$$

(3.1)

where $S$ is a region containing the square and $\mathcal{U}_S$ a suitable set of functions. Neglecting the wave guides, the correct formulation would be to take for $S$ the whole plane and for $\mathcal{U}_S$ functions on the whole plane that decay sufficiently fast, i.e. quasi-confined. Then correct interface conditions result from the index difference in the material square. A confined formulation would be possible by taking for $S$ the material square, and giving suitable boundary conditions on the boundary of the square for functions in $\mathcal{U}_S$. These boundary conditions will involve the Dirichlet-to-Neumann operator of the complement of the material square (see [3]). This DtN-operator is difficult to write down explicitly, and, being a pseudo-differential operator, it would have to be approximated in any numerical method.

Here we will describe a simplified, approximate, formulation in which $S$ is simply a square and $\mathcal{U}_S$ the set of functions that vanish at the boundary: an attractive confined formulation of the original problem. However, the dimension of the square, say with sides of length $L$, does not coincide with the material square that has sides of length $L_{mat}$; $L$ is slightly larger, intuitively
speaking, in order to compensate for the evanescent tails of the field that extend outside the boundaries of the material resonator.

In the figure 3 the situation is demonstrated. The most left picture (fig 3) is a plot of the actual field; shown is also the material boundary, and visible is the evanescent field outside the material square. The second picture (fig 3) from the left shows an exact eigenfunction of the Dirichlet problem on the square with dimension $L$. This solution is explicitly given by a $2:3$ resonance,

$$\sin(2\pi z/L) \sin(3\pi x/L) - \sin(3\pi z/L) \sin(2\pi x/L),$$

and the density plot shows perfect resemblance with the actual field. The same holds true for the value of the resonant frequency: the eigenvalue on the Dirichlet square is in all relevant digits the same as the numerically calculated value. The finding of this explicit expression makes it clear that the physical field is a superposition of two standing waves, which are separately depicted in the two right pictures (fig 3); we will not dwell on this physical interpretation any further here.

![Figure: (3)](image)

In the procedure above, the choice of the value of $L$ is critical. It has been found using the averaged value of the ‘Dirichlet depth’ of each of the modes. Here the Dirichlet depth is defined as the distance to a line parallel to the boundary such that the phase difference of light caused by reflection at the material boundary coincides with the phase difference of light being reflected by a hard mirror (Dirichlet boundary condition) positioned at the parallel line. An alternative method, leading to practically the same result, would be to find this boundary by confining functions from $U_S$ to vanish outside $S$ and to optimize with respect to the position of the (square) boundary.

4. Conclusion

Two examples from integrated optics were described to show how explicit variational methods can be used to achieve direct, constructive formulations.
The increased insight in the functioning of the devices is useful in the actual design process and for the discovery of other devices. Besides this, numerical methods, such as Finite Element methods, can be based on these explicit formulations to obtain efficient and reliable quantitative results for such problems that depend in a sensitive way on the geometry and material parameters.

References


