Variational modelling for integrated optical devices
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Abstract

Variational modelling is the use of a variational structure of a problem to simplify the model or to find approximations of the solutions in a consistent way. In both cases the consistent use of the variational structure consists in restricting the relevant functionals to smaller sets and consider the Euler-Lagrange equation on the restricted set instead of on the original set. One type of restriction may be to specialise the set of phenomena. To find approximate solutions, parameterized manifolds of functions are used to restrict the functional; either low-dimensional manifolds of appropriate 'trial'-functions, or high-dimensional linear subspaces for numerical discretizations.

In these notes another type of restriction will be discussed. We describe how typical problems for all-optical devices in integrated optics have to be considered on unbounded domains. The variational structure is then exploited to confine the problem to a finite domain by restriction to functions that satisfy, or approximate, the equations on the exterior domain. For a typical reflection problem this leads to boundary conditions that are 'transparent' for a-priorily unknown radiation and transmittance, but allow a prescribed influx of light into the structure.

1 Prelim: Macroscopic Maxwell Equations

The Macroscopic Maxwell Equations (MME) in a medium without free charges are given in its standard form by

$$\partial_t \begin{pmatrix} \mathbf{D} \\ \mathbf{B} \end{pmatrix} = \begin{pmatrix} 0 & curl \\ -curl & 0 \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix}$$

where the basic electromagnetic fields are

$\mathbf{E}$: electric field
$\mathbf{H}$: magnetic field

and the variables

$\mathbf{D}$: dielectric displacement
$\mathbf{B}$: magnetic induction

are expressed in $\mathbf{E}, \mathbf{H}$ by so-called *constitutive relations:*

- for propagation in vacuum, $\mathbf{D} = \varepsilon_0 \mathbf{E}, \mathbf{B} = \mu_0 \mathbf{H}$ with ε_0, μ_0constant ($\varepsilon_0 \mu_0 = \frac{1}{c^2}$ with c the speed of light in vacuum);

- for propagation in material, polarization effects are present because of interaction of fields with molecules and electrons; in these lectures we will assume that the magnetic susceptibility vanishes at the relevant optical frequencies, in which case one has

$$\begin{aligned}\mathbf{D} &= \varepsilon_0\mathbf{E}+\mathbf{P}(\mathbf{E})\\ \mathbf{B} &= \mu_0\mathbf{H}\end{aligned}$$

  with polarization $\mathbf{P}$ depending on $\mathbf{E}$ in a way determined by the material properties.

- For lossless materials, to which we will restrict in the following, the constitutive relations can be formulated using constitutive functionals[1]. In particular, a functional $\mathcal{H}$ of $\mathbf{E},\mathbf{H}$ can be found such that

$$\mathbf{D}=\delta_{\mathbf{E}}\mathcal{H}\ ,\ \ \mathbf{B}=\delta_{\mathbf{H}}\mathcal{H} \text{ with } \mathcal{H}=\mathcal{C}(E)+\int\frac{1}{2}\mu_0\mathbf{H}\cdot\mathbf{H}.$$

  For instance, in vacuum, the constitutive functional $\mathcal{C}(E)$ on a domain Ω reads

$$\mathcal{C}(\mathbf{E})=\int\frac{1}{2}\varepsilon_0\mathbf{E}\cdot\mathbf{E}$$

- As a consequence of the variational structure of the constitutive relations, and the fact that (with suitable boundary conditions) the matrix operator $\Gamma=\begin{pmatrix}0 & curl\\ -curl & 0\end{pmatrix}$ is skew-symmetric (since *curl* is symmetric), Maxwell equations can be written down in the following variational form[2]:

$$\partial_t\delta\mathcal{H}=\Gamma\delta\mathcal{E} \text{ with } \mathcal{E}=\int\frac{1}{2}(\mathbf{E}\cdot\mathbf{E}+\mathbf{H}\cdot\mathbf{H}).$$

Poynting vector

Multiplying the Maxwell equations by the fields, one observes the identity:

$$\mathbf{E}\cdot curl\mathbf{H}-\mathbf{H}\cdot curl\mathbf{E}=\mathbf{E}\cdot\partial_t\mathbf{D}+\mathbf{H}\cdot\partial_t\mathbf{B}$$

Using standard vector identity the lhs can be written $-div\,(\mathbf{E}\times\mathbf{H})$; the rhs can be written as a time derivative. For the general setting involving the constitutive functional $\mathcal{H}$, it is easier to integrate over a domain Ω, which then leads to the integrated form of a local conservation law:

$$\int_\Omega div\,(\mathbf{E}\times\mathbf{H})=\partial_t\left[\mathcal{H}-\int_\Omega(\mathbf{E}\cdot\mathbf{D}+\mathbf{H}\cdot\mathbf{B})\right]$$

For instance, in vacuum, the expression in brackets in the rhs reads

$$\mathcal{H}-\int_\Omega(\mathbf{E}\cdot\mathbf{D}+\mathbf{H}\cdot\mathbf{B})=-\int_\Omega\frac{1}{2}(\varepsilon_0\mathbf{E}\cdot\mathbf{E}+\mu_0\mathbf{H}\cdot\mathbf{H})$$

[1] We do not specify here whether these functionals are defined as integrals over the spatial domain or as integrals over the time. We will see below in the case of one spatial dimension that a time-integration may be most natural.

[2] As a dynamical system evolving in time, this is of the form of a Poisson system when the functionals involved are given by integrations over the spatial domain. When they are given by integrals over time, the 'dynamic' interpretation is different, but a variational structure is present. This can be seen by formally writing the equations like

$$\partial_t^{-1}\Gamma\begin{pmatrix}\mathbf{E}\\ \mathbf{H}\end{pmatrix}=\delta\mathcal{H}$$

and, observing that in space-time the operator $\partial_t^{-1}\Gamma$ is symmetric, writing down the Lagrangian for this equation.

and the local conservation law is given by

$$div\,(\mathbf{E}\times\mathbf{H})+\partial_t\left[\frac{1}{2}(\varepsilon_0\mathbf{E}\cdot\mathbf{E}+\mu_0\mathbf{H}\cdot\mathbf{H})\right]=0.$$

This shows that in the simplest cases the conserved density is the 'electro-magnetic' energy; the energy flux density is known as the Poynting vector

$$\mathbf{S}_{Poynting}=\mathbf{E}\times\mathbf{H}$$

Special cases of the Poynting vector will appear regularly in the following.
Monochromatic light
In many cases one is interested to investigate time harmonic solutions (often called CW: Continuous Waves, in the physics literature), with frequency ω that may be prescribed or to be found. Then it is custom to exploit complex notation and write fields like $\mathbf{E}=\frac{1}{2}\hat{\mathbf{E}}e^{-i\omega t}+cc$, where here and in the following, cc denotes 'complex conjugate'. Solutions of this type can only be expected to exist provided the polarization of a time-harmonic field is purely harmonic with the same frequency. Then the equations become

$$-i\omega\begin{pmatrix}\hat{\mathbf{D}}\\ \hat{\mathbf{B}}\end{pmatrix}=\begin{pmatrix}0 & curl\\ -curl & 0\end{pmatrix}\begin{pmatrix}\hat{\mathbf{E}}\\ \hat{\mathbf{H}}\end{pmatrix}$$

which can be written by eliminating the magnetic field like

$$-\omega^2\mu_0\hat{\mathbf{D}}=curl\ curl\hat{\mathbf{E}}.$$

The variational formulation is then retained by using the related constitutive functional:

$$\delta\left[\int\left|curl\hat{\mathbf{E}}\right|^2+\omega^2\mu_0\mathcal{C}(\hat{\mathbf{E}})\right]=0.$$

Integrating the local conservation law over one time-period, there results the spatial conservation of the Poynting vector

$$div\hat{\mathbf{S}}=0\ \text{ for }\ \hat{\mathbf{S}}=\frac{1}{2}\,\mathrm{Re}\left(\hat{\mathbf{E}}\times\hat{\mathbf{H}}^*\right).$$

Applying Gausz' theorem, this shows that for each domain Ω with boundary $\partial\Omega$ (with outward pointing normal $\mathbf{n}$ to the boundary) the total flux through the boundary vanishes:

$$\int_\Omega div\hat{\mathbf{S}}=(\text{Gausz})=\int_{\partial\Omega}\hat{\mathbf{S}}\cdot\mathbf{n}=0.$$

1.1 Restriction to 2 spatial dimensions

In the following we will restrict to two-dimensional (2D) spatial problems (or to 1D). We will think of structures and variables independent of y, and light propagation in the z-direction. Then the total set of equations for the six field components decouple into two sets of equations for three components only, a splitting is so-called TE-modes (transverse electric) and TM-modes (transverse magnetic):

$$\begin{aligned}\text{TE-case}\quad &:\quad \mathbf{E}=(0,E_y,0),\quad \mathbf{H}=(H_x,0,H_z)\\ \text{TM-case}\quad &:\quad \mathbf{E}=(E_x,0,E_z),\quad \mathbf{H}=(0,H_y,0)\end{aligned}$$

Restricting to the TE-case, and assuming that the polarization has also only its y-component non-vanishing, MME's become

$$\begin{aligned} \partial_t D_y &= \partial_z H_x - \partial_x H_z \\ \mu_0 \partial_t H_x &= \partial_z E_y \\ \mu_0 \partial_t H_z &= -\partial_x E_y. \end{aligned}$$

These equations can be reduced to a scalar equation for $E \equiv E_y$, with $D \equiv D_y$, the sME (scalar Maxwell Equation):

$$\textbf{sME}: \quad \mu_0 \partial_t^2 D = \Delta E \equiv \left(\partial_x^2 + \partial_z^2\right) E;$$

in vacuum this leads to the standard wave equation: $\partial_t^2 E = c^2 \Delta E$.
For monochromatic light there results the Helmholtz equation:

$$-\omega^2 \mu_0 \hat{D} = \Delta \hat{E}$$

with variational formulation

$$\delta \left[\int |\nabla \hat{E}|^2 + \omega^2 \mu_0 \mathcal{C}(\hat{E}) \right] = 0.$$

The Poynting vector is given by

$$\mathbf{S} = (E_y H_z, 0, -E_y H_x)$$

and for monochromatic light by

$$\hat{\mathbf{S}} = \frac{-1}{2\omega\mu_0} \operatorname{Im}(\hat{E}_y \partial_x \hat{E}_y^*, 0, \hat{E}_y \partial_z \hat{E}_y^*)$$

Then $div \hat{\mathbf{S}} = 0$ leads to

$$\operatorname{Im}\left(\hat{E}_y \Delta \hat{E}_y^*\right) = 0$$

1.2 Restriction to 1 spatial dimension

With further restriction, uniformity in the x and y-direction, a further simplification is obtained: the MME's become

$$\partial_t D_y = \partial_z H_x, \quad \mu_0 \partial_t H_x = \partial_z E_y \tag{1}$$

and hence

$$\begin{aligned} \text{sME} &: \quad \mu_0 \partial_t^2 D = \partial_z^2 E \\ \text{Helmholtz} &: \quad -\mu_0 \omega^2 D = \partial_z^2 E \\ \text{Poynting vector} &: \quad \mathbf{S} = (0, 0, -E_y H_x) \\ \text{for monochromatic light} &: \quad \hat{\mathbf{S}} = \frac{-1}{2\omega\mu_0} \operatorname{Im}(0, 0, \hat{E}_y \partial_z \hat{E}_y^*) \end{aligned}$$

Then $div \hat{\mathbf{S}} = 0$ leads to

$$\operatorname{Im} \partial_z (\hat{E}_y \partial_z \hat{E}_y^*) = \operatorname{Im}\left(\hat{E}_y \partial_z^2 \hat{E}_y^*\right) = 0$$

2 Intro: Hemholtz equation for planar optical problems

In modern optical telecommunication, all-optical devices are used to manipulate light for various purposes. These (nano-scale) devices exploit interference properties to manipulate the light that is transported to and from the device through waveguides; for instance, a filter will select a specific wavelength from a broad spectrum of light. Characteristic is that these problems have to be modelled on unbounded domains. Although the device (and surrounding region where the changes in light are most essential) is 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.

Remark 1 Consistent numerical algorithms. *The confined variational formulations that we will derive are well-suited to derive numerical discretizations in a consistent way by replacing the continuous functions by a finite dimensional approximation. For instance, using spline-interpolation, algorithms known as Finite Element Methods are obtained.*

When restricting to planar structures, and to materials that are lossless (non-dissipative), nonmagnetic and linear, Mawell's equations reduce for monochromatic light to the inhomogeneous Helmholtz equation; for so-called TE-modes a scalar equation is obtained for the spatially dependent part of the perpendicular electromagnetic field component. Writing $E(x,z;t) = u(x,z)exp(-i\omega t) + cc$ the equation for the (complex valued) spatial dependence reads

$$\Delta u + k^2(x,z)u = 0 \tag{2}$$

The function $k = k(x,z) = k_0 n(x,z)$, where $k_0 = \omega/c$ and c the speed of light in vacuum, contains the (real valued) index of refraction n which is different for different materials, and characterizes the geometry of the device.
At interfaces between different materials, jumps in n between piecewise constant values occur and the weak form of the equation requires continuity of the function u and its normal derivative as interface conditions.
When the material has Kerr-nonlinearity, the equation reads

$$\Delta u + k^2(x,z)u + \gamma|u|^2 u = 0 \tag{3}$$

2.1 Formal variational structure

Formally the variational structure of equation (2) is determined by the critical points of the real- or, alternatively, of the complex-valued functional:

$$\int \left[|\nabla u|^2 - k^2|u|^2\right] \text{ or } \int \left[(\nabla u)^2 - k^2 u^2\right]$$

on the whole plane. In the next applications we show how these can be modified to obtain formulations on bounded domains with appropriate boundary conditions.
For nonlinear materials with Kerr-nonlinearity, solutions of the equation (3) are critical points of the real-valued functional

$$\int \left[|\nabla u|^2 - k^2|u|^2 - \frac{1}{2}\gamma|u|^4\right] .$$

3 Compatibility BC for HE

3.1 General idea

Consider the HE on a domain Ω with boundary $\partial\Omega$, and prescribed BC's at $\partial\Omega$ (partially Neumann and/or Dirichlet) so that a unique solution exists, say U.
Suppose the domain Ω is divided into two domains $\Omega = \Omega_1 \cup \Omega_2$, with a corresponding division of the boundary $\partial\Omega_1 \subset \partial\Omega$ and $\partial\Omega_2 \subset \partial\Omega$. Let Γ denote the common part of the boundary of the two domains.
The aim is to formulate boundary conditions on Γ so that the resulting BVP on Ω_1 has as solution, say u_1 on Ω_1, the restriction of the solution on Ω to Ω_1.
These boundary conditions on Γ will, of course, depend on the boundary conditions on the part of the boundary $\partial\Omega_2$. Stated differently, information of the total solution that is restricted to Ω_2 should be translated to information at Γ such that the problem on Ω_1 is well defined and has the correct solution.
For a given equation, and a given boundary Γ, a set of conditions at Γ will be called *Compatibility Boundary Conditions (CBC)* if they serve the desired aim.
For the case of the Helmholtz equation, the basic ingredient is the following observation.
A solution u_1 on Ω_1 and a solution u_2 on Ω_2 can be matched into a smooth solution on the whole domain Ω if and only if at the boundary Γ the following interface conditions are satisfied:

$$\begin{aligned} u_1 &= u_2 \text{ on } \Gamma \text{ (continuity)} \\ \partial_n u_1 &= \partial_n u_2 \text{ on } \Gamma \text{ (continuity of normal derivative)} \end{aligned}$$

(Here, n is the normal to Γ pointing *outwards* the domain Ω_1). This shows the way how to 'construct' CBC's as we will now describe.

Let $U_2(\phi)$ be the solution of HE with given BC at $\partial\Omega_2$ which has the value ϕ at Γ :

$$U_2(\phi) = \phi \text{ at } \Gamma.$$

Consider the normal derivative of this solution on Γ, and define in this way a mapping $\mathcal{D}$:

$$\mathcal{D} : \phi \to \partial_n U_2(\phi)$$

called (for obvious reasons) the *Dirichlet-to-Neumann (DtN) operator.* Then we have:

Claim 2 *If U_1 is a solution of HE on the subdomain Ω_1 which satisfies the given BC at $\partial\Omega_1$ and which satisfies, moreover, the following condition at Γ :*

$$\partial_n(u) = \mathcal{D}(u) \text{ at } \Gamma \tag{4}$$

then U_1 is a solution that can be extended to the whole domain Ω which satisfies the BC at $\partial\Omega$. We will call (4) a Compatibility Boundary Condition *at Γ.*

Indeed, suppose that the value of the solution U_1 is denoted by $U_1 = \psi$ at Γ. Then 'calculate' the solution, say V, of HE on Ω_2 with specified BC at $\partial\Omega_2$ and with $V = \psi$ at Γ. Then $V = \psi = U_1$ on Γ. But also

$$\partial_n V = (\text{by definition of } \mathcal{D}) = \mathcal{D}(\psi) = (\text{by CBC}) = \partial_n(U_1) \text{ on } \Gamma,$$

and so U_1 and V are the restrictions of one smooth solution on the whole domain Ω.
To be applicable, we have to find the DtN-operator $\mathcal{D}$. Note that this operator will depend on the specified boundary-condition at $\partial\Omega_2$. Unfortunately, in most interesting cases, the operator cannot be found explicitly and we will have to look for approximations.

Example 3 *Consider the simple BVP on* $[-\ell, 1]$

$$\begin{aligned} -\partial_z^2 u &= 0 \text{ on } [-\ell, L] \\ u(-\ell) &= H; u(L) = 0 \end{aligned}$$

Suppose the interval is splitt like $[-\ell, 1] = [-\ell, 0] \cup [0, L]$*. Any solution on* $[-\ell, 0]$ *is of the form* $u(z) = a(z + \ell) + H$*, for some* a*. Since* $u(0) = a\ell + H$*, and* $\partial_z(0) = a$*, this leads to the DtN operator at the point* $z = 0$*:*

$$\mathcal{D}(u_0) = -(u_0 - H)/\ell \text{ at } z = 0$$

The solutions on $[0, 1]$ *with* $u(1) = 0$ *are of the form* $u(z) = \alpha(z - L)$ *and satisfy* $u(0) = -\alpha L$*,* $\partial_z u(0) = \alpha$*. The one satisfying the CBC* $\partial_z u = -\mathcal{D}(u)$ *at* $z = 0$ *has to satisfy* $\alpha L = (-\alpha - H)/\ell$ *leading to* $\alpha = -H/(\ell + L)$*. This is the solution on* $[0, L]$ *that can indeed be smoothly continued to the solution on the whole interval satisfying the correct boundary conditions at* $z = -\ell$*,* $z = L$*.*

3.2 Variational formulation

Considering the same problem as above, we split the functional

$$\mathcal{L}(u) := \int_\Omega \left[(\nabla u)^2 - k^2 u^2\right]$$

in two functionals corresponding to the division of the domain:

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2, \text{ with } \mathcal{L}_j(u) = \frac{1}{2}\int_{\Omega_j} \left[(\nabla u)^2 - k^2 u^2\right]$$

For a function u on Ω, the first variation of the functionals, for variation v_j in the domain Ω_j are given by

$$\delta\mathcal{L}_j(u; v_j) = \int_{\Omega_j} \left[(\nabla u)(\nabla v_j) - k^2 u v_j\right] = \int_{\Omega_j} \left[(-\Delta u - k^2 u)v_j\right] + \int_{\partial\Omega_j} \left[(\partial_n u)\, v_j\right] + \int_{\Gamma_j} \left[\left(\partial_{n_j} u\right) v_j\right]$$

with $\Gamma_1 = \Gamma_2 = \Gamma$ and with outward pointing normal, so $n := n_1 = -n_2$ on Γ
Let u on Ω be composed of functions u_1 on Ω_1 and u_2 on Ω_2 with u_j satisfying the equation in Ω_j and the boundary condition at $\partial\Omega_j$, then for all variations v_j that are consistent with the boundary conditions on $\partial\Omega_j$ but 'free' at Γ, it holds that

$$\Sigma_{j=1,2}\left\{\int_{\Omega_j} (-\Delta u - k^2 u)v_j + \int_{\partial\Omega_j} (\partial_n u)\, v_j\right\} = 0.$$

If we require that the solution should be continuous across Γ, $u_1 = u_2$ at Γ, the admissible variations should be continuous across Γ, $v_1 = v_2$ on Γ, the vanishing of the first variation requires

$$\int_{\Gamma_1} (\partial_n u)\, v_1 - \int_{\Gamma_2} (\partial_n u)\, v_2 = 0$$

and this then implies continuity of the normal derivative across Γ.
Using the above defined DtN-operator here, we can write in fact

$$\delta\mathcal{L}_2(u; v) = -\int_\Gamma \mathcal{D}(u) v$$

Hence the correct formulation on Ω_1 is found from

$$\delta\mathcal{L}_1(u;v) - \int_\Gamma \mathcal{D}(u)v = 0 \tag{5}$$

for the function u that satisfies the prescribed boundary condition at $\partial\Omega_1$ and that is free at Γ, and for which the expression vanishes for all admissible variations v.

The formulation (5) as given is not immediately recognized as originating from a variational principle defined on Ω_1. Yet it is, as can be seen as follows.
Define the 'value-functional' of the problem on Ω_2 as the value of the functional for solutions that has value ψ on Γ :

$$V(\psi) = \text{Crit } \{\mathcal{L}_2(u) \mid u \text{ prescribed at } \partial\Omega_2, \quad u = \psi \text{ on } \Gamma\} .$$

Note that this is a boundary functional, defined for functions on Γ. To prevent possible confusion in the following, we emphasize that the value function is defined with prescribed (fixed) conditions at the boundary part $\partial\Omega_2$.Then, from the first variation of $\mathcal{L}_2$ we have that for this boundary functional

$$\delta V(\psi;\delta\psi) = -\int_\Gamma \mathcal{D}(\psi)\delta\psi.$$

This means that we have:

Proposition 4 *The DtN-operator for the problem is equal to (minus) the variational derivative of the value function:*

$$\mathcal{D}(\psi) = -\delta\mathrm{V}(\psi); \tag{6}$$

here, in the natural way, the first variation $\delta\mathrm{V}(\psi)$ is defined with the innerproduct on the boundary Γ.

This then leads to the immediate result:

Proposition 5 *The variational problem*

$$\textit{Crit } \{\mathcal{L}_1(u) + \mathrm{V}(u|_\Gamma) \mid u \textit{ prescribed at } \partial\Omega_1, \quad u \textit{ free at } \Gamma\} \tag{7}$$

leads to (5) as the first variation,and therefore to the BVP on Ω_1 with the CBC on Γ.

Example 6 *Consider the same simple BVP as above on $[-\ell, L]$*

$$\begin{aligned} -\partial_z^2 u &= 0 \text{ on } [-\ell, L] \\ u(-\ell) &= H; \quad u(L) = 0 \end{aligned}$$

now in the variational setting. Split the integrals

$$\mathcal{L}_-(u) = \int_{-\ell}^0 \frac{1}{2}\left|\partial_z u\right|^2, \mathcal{L}_0(u) = \int_0^L \frac{1}{2}\left|\partial_z u\right|^2$$

The value function of the left interval problem, as function of the value u_0 at $z=0$ is given by

$$\mathcal{V}_-(u_0) = (\frac{1}{2}u_0^2 - Hu_0)/\ell$$

and as stated in general above, the DtN-operator is indeed found from

$$\mathcal{D}(u_0) = -\frac{\partial \mathcal{V}_-}{\partial u_0}.$$

Hence the correct restricted problem on $[0, L]$ *is found as critical points of*

$$Crit\ \{\mathcal{L}_0(u) + \mathcal{V}_-(u_0)\ \mid u(L) = 0\}\ ;$$

in particular the correct boundary value at $z = 0$ *is found from the variations of the endvalue* u_0 *at* $z = 0$.

Remark 7 *The formulation of the DtN-operator as the variational derivative of the boundary functional leads to a possible method to approximate the DtN operator in case it cannot be found explicitly (which is the usual case). This is comparable to the problem in surface waves on a layer of incompressible, irrotational fluid. There the kinetic energy is defined as a boundary-functional, the boundary being the free surface described with a function* $\eta = \eta(x)$, *as the value function*

$$K(\eta, \phi) = \min_{\Phi} \left\{ \int dx \int^{\eta(x)} \frac{1}{2} |\nabla \Phi|^2 \, dz \ \middle| \ \Phi(x, z = \eta) = \phi \right\}$$

Also in this case there is no possibility to find the functional in an explicit way; approximations lead to explicit functionals which then give rise to approximate models of Boussinesq (or KdV) type. Just as in this case, it is to be expected that approximation of the boundary-functional and then using this approximation in the variational formulation will lead to 'better', because variationally consistent, *model equations.*

4 Transparent-Influx BC for confinement

4.1 General idea

In 2(3)D-problems from integrated optics the situation is more complicated since then the problem is originally defined on the whole real plane (space). Then, in analogy with the bounded example from above, with Ω a bounded domain, boundary conditions are sought such that the 'interior' solution u_{int} inside Ω can be smoothly extended to an 'exterior' solution u_{ext} in the complementary domain $\Omega^c = \mathcal{R}^2 \backslash \Omega$. (Note the change in notation: Ω_1 above is now Ω, and Ω_2 is now Ω^c; also, the boundary of the domain above is now in fact the boundary 'at infinity' of Ω^c.
Let Γ denote the boundary of Ω (and let n be the outward pointing normal) then we want to satisfy the conditions

$$u_{int} = u_{ext} \text{ and } \partial_n u_{int} = \partial_n u_{ext} \text{ at } \Gamma.$$

Replacing 'boundary conditions' at infinity, the exterior solution will have to satisfy certain influx and/or outflux conditions in general. More precisely, suppose there is given an external incoming field, that is specified by its value and flux at the boundary Γ :

$$u^{in} = f \ \text{ and } \partial_n u^{in} = F \ \text{ on } \Gamma$$

To find boundary conditions on Γ that are 'compatible' now means BC's that guarantee that a solution inside Ω can be extended to a solution on the whole plane, satisfying the in/outflux conditions.

For reasons that will become clear soon, we call such boundary conditions *Transparent-Influx BC's (TIBC)*. To that end we now introduce two types of *Dirichlet-to-Neumann operators*:

$$\begin{aligned}\mathcal{D}^+(\phi) &= \partial_n U|_\Gamma \text{ with } U \text{ solution of extHE-OUT with } U_\Gamma = \phi\\ \mathcal{D}^-(\phi) &= \partial_n U|_\Gamma \text{ with } U \text{ solution of extHE-IN with } U_\Gamma = \phi\end{aligned}$$

where:

ExtHE-OUT : exterior HE with OUTgoing Sommerfeld
ExtHE-IN: exterior HE with INcoming Sommerfeld

With this notation we can specify what is meant by an 'incoming field', namely that it corresponds to a solution u^{in} of extHE-IN, with

$$u^{in}\big|_\Gamma = f \text{ and } \mathcal{D}^-(f) = F.$$

Write the total solution u^c on the unbounded complement Ω^c as a sum of parts that satisfy the incoming and outgoing Sommerfeld condition:

$$u^c = u^{in} + u^{out}$$

Then a solution u_Ω in the interior has to satisfy

$$\partial_n u_\Omega = \partial_n u^c = \mathcal{D}^+(u^{out}\big|_\Gamma) + \mathcal{D}^-(u^{in}\big|_\Gamma)$$

Using continuity at the boundary, we can write for the actual value of the solution at Γ : $u_\Omega|_\Gamma = f + u^{out}|_\Gamma$. However u^{out} is not known; it has an obvious interpretation as the *radiation.* Therefore we eliminate it in the following chain of equalities by expressing it in the value of the total solution at the boundary:

$$\begin{aligned}\partial_n u_\Omega &= \partial_n u^c = \mathcal{D}^+(u^{out}\big|_\Gamma) + \mathcal{D}^-(u^{in}\big|_\Gamma) =\\ &= \mathcal{D}^+(\big(u_\Omega - u^{in}\big)\big|_\Gamma) + F\\ &= \mathcal{D}^+(u_\Omega|_\Gamma) - \mathcal{D}^+(u^{in}\big|_\Gamma) + \mathcal{D}^-(u^{in}\big|_\Gamma)\end{aligned}$$

In this way we get as *TIBC*

$$\partial_n u_\Omega - \mathcal{D}^+(u_\Omega|_\Gamma) = F - \mathcal{D}^+(f).$$

This is a relation for the function u_Ω between its value and its normal derivative at the boundary (on the left hand side) and the specified influx conditions at the right hand side. In the special case when there is no incoming field, we have a boundary condition that is transparent for outgoing waves:

$$\partial_n u - \mathcal{D}^+(u) = 0$$

4.2 Variational formulation

With obvious adaptations, and some additional precautions for the unboundedness of the domain, the same steps can be done as in the case of a bounded domain.
Consider the unbounded problem as above, and split the formal functional on the whole plane

$$\frac{1}{2}\int_{\mathcal{R}^2}\left[(\nabla u)^2 - k^2u^2\right] = \mathcal{L}(u) + \mathcal{L}_c(u) := \frac{1}{2}\int_\Omega \left[(\nabla u)^2 - k^2u^2\right] + \frac{1}{2}\int_{\Omega^c}\left[(\nabla u)^2 - k^2u^2\right]$$

We have to recognize that this may be only a formal way of writing since the functional on the unbounded domains may not be bounded or not be defined (as a sensible limit of integrals over increasingly larger domains). However, for any function u on $\mathcal{R}^2$, the first variation of each of the functionals exist if we require the variations on the unbounded domain to be admissible provided they vanish sufficiently fast at infinity. Then, for admissible variations we have

$$\begin{aligned} \delta\mathcal{L}(u;v) &= \int_\Omega \left[(\nabla u)\,(\nabla v) - k^2 uv\right] = \int_\Omega \left[(-\Delta u - k^2 u)v\right] + \int_\Gamma \left[(\partial_n u)\,v\right] \\ \delta\mathcal{L}^c(u^c;v^c) &= \int_{\Omega^c} \left[(\nabla u^c)\,(\nabla v^c) - k^2 u^c v^c\right] = \int_{\Omega^c} \left[(-\Delta u^c - k^2 u^c)v^c\right] - \int_\Gamma \left[(\partial_n u^c)\,v^c\right] \end{aligned}$$

with outward pointing normal n on Γ. If we require continuity across Γ, $u = u^c$ at Γ, the requirement that the the first variation

$$\delta\mathcal{L}(u;v) + \delta\mathcal{L}^c(u^c;v^c)$$

vanishes for all admissible variations that are continuous across Γ leads to the correct equation in Ω and to the interface conditions at Γ: $u = u^c$ and $\partial_n u = \partial_n u^c$ at Γ, where u^c is a solution in the exterior.

Using the above defined DtN-operators, the correct formulation on Ω for the influx problem is found from

$$\delta\mathcal{L}(u;v) - \int_\Gamma \mathcal{D}^+(u|_\Gamma)v + \int_\Gamma \left[\mathcal{D}^+(\,u^{in}\big|_\Gamma) - \mathcal{D}^-(\,u^{in}\big|_\Gamma)\right] v = 0 \tag{8}$$

for all admissible variations v.

The formulation (8) can be obtained from a variational principle defined on Ω by introducing value functions for outgoing and incoming waves which are related to the valuefunction on the unbounded region.

5 1D Reflection/transmittance problem

Consider the simple example of a 1-dimensional scattering problem. Assume that (arbitrary) index variations are restricted to an interval $z \in (0, L)$ while outside this interval $k(z)$ is constant, say $k(z) = k_-$ for $z < 0$ and $k(z) = k_+$ for $z > L$. An incoming wave from the left is considered with amplitude A, and no incoming waves from the right. Reflected and transmitted waves with a priory unknown reflection (r) and transmittance (t) coefficient have to be taken into account, so

$$u = A\exp(ik_- z) + r\exp(-ik_- z) \text{ for } z < 0$$

and

$$u = t\exp ik_+(z - L) \text{ for } z > L.$$

5.1 Transparent-Influx BC's

We now transform the problem to a confined problem by deriving the TIBC's.

At the left, $z < 0$, we have an incoming wave $Ae^{ik_0 z}$, (travelling to right, hence incoming) and hence

$$\begin{aligned} u^{in}(z &= 0) = A \\ \partial_n u(z &= 0) = -\partial_z u(z = 0) = -ik_- A \end{aligned}$$

For this simple problem we can easily calculate $\mathcal{D}^+$ at $z = 0$:

$$\begin{aligned}
\mathcal{D}^+(\alpha) &= -\partial_z(\alpha e^{-ik_- z})|_{z=0} = ik_-\alpha, \\
\text{so } \mathcal{D}^+(u) &= ik_- u \text{ at } z = 0.
\end{aligned}$$

Hence we have as Influx-Transparent- Bdy-cond: $\partial_n u - ik_- u = -ik_- A - ik_- A = -2ik_- A$, i.e.

$$\partial_z u + ik_- u = 2ik_- A$$

In the same way, for the transparent boundary condition at $z = L$ we find

$$\partial_z u - ik_+ u = 0 \text{ at } z = L$$

Example 8 *If the index is constant over the whole real line, $k(z) = k_0$ constant, the influx at $z = 0$ of the wave $Ae^{ik_0 z}$, should be the same outflux at $z = L$, which indeed satisfies the TIBC's:*

$$\begin{aligned}
\partial_z u + ik_0 u &= 2ik_0 A \text{ at } z = 0, \\
\partial_z u - ik_0 u &= 0 \text{ at } z = L
\end{aligned}$$

When a mirror is placed at $z = L$, and hence there is total reflection at $z = L$, with boundary condition $u = 0$ at $z = L$,the solution is

$$u = Ae^{ik_0 z} - Ae^{ik_0(2L-z)}$$

This solution indeed satisfies the TIBC at $z = 0$

$$\partial_z u + ik_0 u = 2ik_0 A \text{ at } z = 0;$$

observe that the reflected wave is nicely transmitted through $z = 0$; the value of the solution at $z = 0$ is $u(0) = A\left(1 - e^{2Lik_0}\right)$, and the Poynting quantity is zero for this standing wave at the left.

5.2 Variational formulation

The confined problem derived above:

$$\begin{aligned}
\partial_z^2 u + k^2(z)u &= 0, \\
\partial_z u + ik_- u &= 2ik_- A \text{ at } z = 0, \\
\partial_z u - ik_+ u &= 0 \text{ at } z = L
\end{aligned}$$

corresponds to the equation and natural boundary conditions for critical points of the functional

$$\mathcal{L}(u) = \int_0^L \frac{1}{2}\left[(\partial_z u)^2 - k^2 u^2\right] dz - \frac{1}{2} ik_- u(0)^2 - \frac{1}{2} ik_+ u(L)^2 + 2ik_- Au(0).$$

This follows with the standard reasoning from the vanishing of the first variation:

$$\begin{aligned}
\delta\mathcal{L}(u; v) &= \int_0^L \left[(\partial_z u)(\partial_z v) - k^2 uv\right] dz - ik_- u(0)v(0) - ik_+ u(L)v(L) + 2ik_- Av(0) \\
&= \int_0^L \left[-\partial_z^2 u - k^2 u\right] v dz + (\partial_z u)v|_{z=0}^{z=L} - ik_- u(0)v(0) - ik_+ u(L)v(L) + 2ik_- Av(0)
\end{aligned}$$

Restricting first to test functions on the interval $[0, L]$ shows that the correct Helmholtz equation is obtained. Hence, there remains the vanishing of the boundary variations:

$$(\partial_z u)v|_{z=0}^{z=L} - ik_- u(0)v(0) - ik_+ u(L)v(L) + 2ik_- Av(0) = 0$$

From this, arbitrary variations of the boundary value $v(0)$ leads to $-\left(\partial_z u\right)|_{z=0} - ik_- u(0) + 2ik_- A = 0$ and arbitrary variations of the boundary value $v(L)$ to: $\left(\partial_z u\right)|_{z=L} - ik_+ u(L) = 0$, which are the required TIBC's.

Remark 9 *Note that we didn't specify the interior structure. Only for simple structures explicit solutions can be found, for instance, with transfer-matrix techniques when k is piecewise constant. Well known examples are gratings, when the index changes periodically. Above, the emphasis has been on the procedure to derive the confined formulation, which can also (in particular) be exploited for numerical discretizations for* any *internal index-variation.*

Exercise 10 *Suppose the index is a constant k_0 in the interior interval.*

1. *Calculate explicitly the solution by matching the general solutions in the three separate intervals using the interface conditions.*
2. *Show that the solution satisfies the TIBC's, and that it indeed can be found by only solving the problem on the bounded interval with the TIBC's.*
3. *Considering the reflection and transmission, determine the length of the structure for which the transmittance is minimal or maximal.*

6 Guided modes: confinement to non-standard eigenvalue problem

Consider a similar index structure as above, now as part of a planar problem that is uniform in the orthogonal x-direction. Assuming $k(z) > max(k_-, k_+)$, this is the model of a straight wave guide in the x-direction. Then the interest is to find guided modes, which are x-periodic waves that are 'guided' in the sense of vanishing in the z-direction:

$$u(x, z) = \phi(z) \exp(i\beta x).$$

This leads to an eigenvalue problem for the profile function $\phi(z)$ and the so-called propagation-constant β:

$$\partial_z^2 \phi + (k^2(z) - \beta^2)\phi(z) = 0, \quad \phi(z) \to 0 \text{ for } z \to \pm\infty.$$

For simplicity we will restrict in the following to symmetric wave guides, $k_- = k_+$ for $|z| > L$ and we will look only for symmetric modes.
For the principal eigenfunction and -value of this eigenvalue problem, a constrained variational formulation on the half-infinite real axis can be given. With a convenient, inessential, normalization for the eigenfunction, this reads

$$-\beta^2 = \min_{\phi} \left\{ \int_0^{+\infty} \left[(\partial_z \phi)^2 - k^2 \phi^2 \right] dz \,\middle|\, \int_0^{+\infty} \phi^2 dz = 1, \phi(z) \to 0 \text{ for } z \to \infty \right\} \tag{9}$$

Exploiting the fact that the solution in the uniform exterior can be written down as an exponentially decaying function depending on the (unknown) value of β, the variational formulation leads to a confined, unconstrained formulation in which the eigenvalue has to be varied as well. The result is (using the notation $\partial_z \psi = \psi_z$)

$$\min_{\psi, \tilde{\beta}} \left\{ \int_0^L \left[\psi_z^2 + (\tilde{\beta}^2 - k^2)\psi^2 \right] dz + \psi(0)^2 \sqrt{\tilde{\beta}^2 - k_-^2} + \psi(L)^2 \sqrt{\tilde{\beta}^2 - k_+^2} - \tilde{\beta}^2 \right\}.$$

Only in the simplest cases, if k is piecewise constant, the guided modes can be found explicitly.

The details of the derivation of the confined formulation are as follows.

Take any point outside the wave guide, say $z = B \geq L$; we will split the interval $[0, \infty)$ in a bounded interior and unbounded exterior: $[0, \infty) = [0, B] \cup [B, \infty)$. In the exterior domain we use the fact that we know the solution if the eigenvalue, say $\tilde{\beta}$, and the value Φ of the field at the point $z = B$ would be known. Then we match this exterior solution to the yet unknown solution ψ in the interior, requiring only continuity of the solution at $z = B$, hence we put $\Phi = \psi(B)$. So, trial functions are taken to be of the form:

$$\phi(z) = \begin{cases} \psi(z) & \text{for } z \in [0, B] \\ \psi(B) \exp(-\sqrt{\tilde{\beta}^2 - \omega^2 n_0^2}(x - B)) & \text{for } z > B. \end{cases}$$

The part of the integral over the exterior domain $\int_B^\infty \left[\partial_z \phi^2 - \omega^2 n^2 \phi^2\right] dz$ is first reduced by partial integration and then by using the fact that the function satisfies the correct equation there. This leads to

$$\begin{aligned} \int_B^\infty \left[\phi_z^2 - k_+^2 \phi^2\right] dz &= \int_B^\infty \left[-\partial_z^2 \phi - k_+^2 \phi\right] \phi dz - \left[\phi \partial_z \phi\right]_{z=B} \\ &= -\tilde{\beta}^2 \int_B^\infty \phi^2 dz + \psi(B)^2 \sqrt{\tilde{\beta}^2 - k_+^2} \end{aligned}$$

With the normalization $1 = \int_0^\infty \phi^2 = \int_0^B \psi^2 + \int_B^\infty \phi^2$ we arrive for the integral over the total domain at

$$\begin{aligned} \int_0^\infty \left[\phi_z^2 - k^2 \phi^2\right] dz &= \int_0^B \left[\partial_z \psi^2 - k^2 \psi^2\right] dz \\ &\quad + \psi(B)^2 \sqrt{\tilde{\beta}^2 - k_+^2} - \tilde{\beta}^2 \left(1 - \int_0^B \psi^2\right) \end{aligned}$$

$$= \int_0^B \left[\psi_z^2 + (\tilde{\beta}^2 - k^2)\psi^2\right] dz + \psi(B)^2 \sqrt{\tilde{\beta}^2 - k_+^2} - \tilde{\beta}^2$$

With this result we can transform the original constrained eigenvalue formulation to the following unconstrained formulation, where now the 'variables' to be varied are the function ψ on the confined interval, and the unknown parameter $\tilde{\beta}$:

$$\begin{aligned} &\min_\phi \left\{ \int_0^\infty \left[\phi_z^2 - k^2 \phi^2\right] \;\middle|\; \int_0^\infty \phi^2 = 1 \;,\; \phi \to 0 \;\text{ for } z \to \infty \right\} = \\ &\min_{\psi, \tilde{\beta}} \left\{ \int_0^B \left[\psi_z^2 + (\tilde{\beta}^2 - k^2)\psi^2\right] dz + \psi(B)^2 \sqrt{\tilde{\beta}^2 - k_+^2} - \tilde{\beta}^2 \right\} \end{aligned} \tag{10}$$

Observe that the correct Euler-Lagrange equation and the natural boundary condition at $z = 0$ are found:

$$\begin{aligned} \partial_z^2 \psi + k^2 \psi &= \tilde{\beta}^2 \psi \text{ for } z \in (0, B) \\ \partial_z \psi &= 0 \text{ at } z = 0 \end{aligned} \tag{11}$$

Moreover, at $z = B$, variations of the free end value $\psi(B)$ leads to the natural boundary condition

$$\partial_z \psi = -\sqrt{\tilde{\beta}^2 - k_+^2} \psi \text{ at } z = B_-. \tag{12}$$

This is a boundary condition for the 'interior' solution (indicated by writing B_-). For the exterior solution a similar relation holds:

$$\partial_z \phi = -\sqrt{\tilde{\beta}^2 - k_+^2}\,\phi \text{ at } z = B_+.$$

Since we required $\phi(B) = \psi(B)$, it follows that also the derivatives are the same:

$$\phi(B) = \psi(B) \text{ and } \partial_x \phi(B) = \partial_x \psi(B).$$

This means that the interior and the exterior solution are matched to make one genuine solution on the whole real line since both interface conditions at $z = B$ are satisfied. Resuming, we can say that we have reduced the problem on the whole real line (9) to the variational formulation (10) on a bounded domain.

Remark 11 *Observe that the variational formulation (10) still has the character of a minimization problem. The optimal value, the eigenvalue to be found* $-\beta^2$*, is actually equal to* $-\tilde{\beta}^2$ *where* $\tilde{\beta}$ *is the solution of the variational problem, i.e. the optimal value* $\tilde{\beta}$ *is the eigenvalue to be found.*
Formulating the results for the differential equation, we observe that in the interior domain we look for a solution and a value $\tilde{\beta}$ *such that (11) is satisfied together with the boundary condition (12). This boundary condition for the interior problem is recognized as a* transparent boundary condition *which makes it possible to replace the unbounded problem to a BVP on a bounded interval.*
Actually, the position of the point $z = B$ *in the above has been 'arbitrary' outside the wave guide, since for* $z > B$ *the solution was determined by the exterior value* k_+*. This makes it clear that there is no objection to take* $B = L$*, just the boundary of the wave guide. For numerical purposes this is the most optimal way to do.*

Exercise 12 *Formulate the problem above by using a suitably defined value-function for the problem on* $z > L$*.*

Exercise 13 *Derive the confined formulation for confined modes of a non-symmetric wave guide.*

Exercise 14 *Reflection in a single-mode waveguide.*
Consider a straight waveguide which is homogeneous in the x*-direction except in an interval* $x \in [0, \ell]$ *in which waves will be partly reflected. Assume that in the homogeneous region the waveguide is uni-modal.*
Consider the case that a single mode is influxed form $x < 0$*, with specified amplitude* A *In* $[0, \ell]$ *partial reflection may occur; suppose that all reflection and transmission is into the single guided mode, at the left and right. Formulate the confined problem on* $[0, \ell]$ *with TIBC s at* $x = 0, x = \ell$*, and give the confined variational formulation.*

Exercise 15 *A KdV-soliton (symmetric at* $x = 0$ *) satisfies for some* $\lambda > 0$ *the BVP*

$$\begin{aligned} \partial_x^2 u + u^2 &= \lambda u, \quad x > 0 \\ \partial_x u &= 0 \text{ at } x = 0, \quad u \to 0 \text{ for } x \to \infty \end{aligned}$$

or, equivalently, is a critical point of

$$Crit \left\{ \int_0^\infty \left[\frac{1}{2}\phi_x^2 + \lambda \phi^2 - \frac{1}{3}\phi^3 \right] \;\middle|\; \phi \to 0 \;\; for \; x \to \infty \right\}.$$

(Verify with phase-plane analysis that such a solution indeed exists for given $\lambda > 0$*).*
Since $u \to 0$ *for* $x \to \infty$ *we have approximately* $\partial_x^2 u - \lambda u = 0$ *for large* x *and we could approximate the solution for large* L *by*

$$u_a(x) = u(L) \exp\left[-\sqrt{\lambda}(x - L)\right] \; for \; x > L \tag{13}$$

To look for a confined formulation of the original BVP, this may lead one to conclude to take as approximate BC at $x = L$

$$\partial_x u = -\sqrt{\lambda} u \text{ at } x = L. \tag{14}$$

1. *Use energy-conservation of the equation to derive an exact expression for a relation between the derivative and the function at each point. Note that if this relation is used, an exact confinement can be achieved! Stated differently,* this relation defines an exact, NONLINEAR TBC, i.e. the exact DtN-operator can be found!

2. *Investigate the error (as function of L) made by taking instead the BC (14) .*

3. *Define an approximation for the value function for the functional on* $[L, \infty)$ *by substituting the approximate solution:*

$$\mathcal{V}_a(u(L)) = \left\{ \int_L^\infty \left[\frac{1}{2}\phi_x^2 + \lambda\phi^2 - \frac{1}{3}\phi^3 \right] \;\middle|\; \phi = u_a = u(L) \exp\left[-\sqrt{\lambda}(x - L) \right] \right\}.$$

   Take as TBC

$$\partial_x u = \frac{\partial \mathcal{V}_a}{\partial u(L)}$$

   and show that this produces a better TBC than (14).

4. *Explain this additional 'variational' accuracyf rom the observation that a first order error in the solution, produces a second order error in the valuefunction because the value of thefunctional is evaluated near a critical value (the first variation vanishes).*

Exercise 16 *Do a similar investigation as above for the KdV-soliton with prescribed norm* $\gamma > 0$*, so now a nonlinear eigenvalue problem:*

$$Crit \left\{ \int_0^\infty \left[\frac{1}{2}\phi_x^2 - \frac{1}{3}\phi^3 \right] \;\middle|\; \int_0^\infty \phi^2 = \gamma \;,\; \phi \to 0 \;\; for \; x \to \infty \right\}$$

7 Summary... ?

For a bounded domain Ω divided into two subdomains with common boundary Γ; functions $u \in U$ are supposed to satisfy Bc's at $\partial\Omega$ and functions on Ω are composed of functions on the two subdomains

$$u = \begin{cases} u_1 & \text{in } \Omega_1 \\ u_2 & \text{in } \Omega_2 \end{cases}$$

and the functional on Ω is written as the sum of functionals defined on the two subdomains: $\mathcal{L}(u) = \mathcal{L}_1(u_1) + \mathcal{L}_2(u_2)$. Then verify the following chain

$$\begin{aligned}
& \text{Crit } \{ \mathcal{L}(u) \mid u \in U \} \\
= \; & \text{Crit } \{ \mathcal{L}_1(u_1) + \mathcal{L}_2(u_2) \mid u_1 = u_2 \text{ on } \Gamma \} \\
= \; & \text{Crit }_{\psi_1 = \psi_2} \; [\text{Crit } \{ \mathcal{L}_1(u_1) \mid u_1 = \psi_1 \text{ on } \Gamma \} + \text{Crit } \{ \mathcal{L}_2(u_2) \mid u_2 = \psi_2 \text{ on } \Gamma \}] \\
= \; & \text{Crit }_{\psi_1 = \psi_2} \; [\text{Crit } \{ \mathcal{L}_1(u_1) \mid u_1 = \psi_1 \text{ on } \Gamma \} + \mathcal{V}(\psi_2)] \\
= \; & \text{Crit } \{ \mathcal{L}_1(u_1) + \mathcal{V}_2(u_1|_\Gamma) \mid u_1 \}
\end{aligned}$$

with value functional

$$\mathcal{V}_2(\psi) = \text{Crit } \{ \mathcal{L}_2(u_2) \mid u_2 = \psi \text{ on } \Gamma \}.$$

Similarly for constrained problems:

$$\begin{aligned}
& \text{Crit } \{ \mathcal{L}(u) \mid \mathcal{K}(u) = \gamma \} \\
= \; & \text{Crit } \{ \mathcal{L}_1(u_1) + \mathcal{L}_2(u_2) \mid u_1 = u_2 \text{ on } \Gamma,\ \mathcal{K}_1(u_1) = \gamma_1, \mathcal{K}_2(u_2) = \gamma_2,\ \} \\
= \; & \text{Crit }_{\psi_1 = \psi_2; \gamma_1 + \gamma_2 = \gamma} \begin{bmatrix} \text{Crit } \{ \mathcal{L}_1(u_1) \mid u_1 = \psi_1 \text{ on } \Gamma,\ \mathcal{K}_1(u_1) = \gamma_1 \} \\ + \text{ Crit } \{ \mathcal{L}_2(u_2) \mid u_2 = \psi_2 \text{ on } \Gamma,\ \mathcal{K}_2(u_2) = \gamma_2 \} \end{bmatrix} \\
= \; & \text{Crit }_{\psi_1 = \psi_2; \gamma_1 + \gamma_2 = \gamma} \left[\text{Crit } \{ \mathcal{L}_1(u_1) \mid u_1 = \psi_1 \text{ on } \Gamma,\ \mathcal{K}_1(u_1) = \gamma_1 \} + \mathcal{V}(\psi_2; \gamma_2) \right] \\
= \; & \text{Crit } \{ \mathcal{L}_1(u_1) + \mathcal{V}_2(u_1|_\Gamma ; \gamma - \gamma_1) \mid \mathcal{K}_1(u_1) = \gamma_1 \}
\end{aligned}$$

with value functional

$$\mathcal{V}_2(\psi; \mu) = \text{Crit } \{ \mathcal{L}_2(u_2) \mid u_2 = \psi \text{ on } \Gamma,\ \mathcal{K}_2(u_2) = \mu \}.$$

In principle, the same analysis is possible for problems on the plane divided in a bounded domain and the complementary unbounded domain; but note that then BC's 'at infinity' may cause problems in the definitions of the value-functionals when the solutions don't vanish at infinity, as for transmission problems.

Exercise 17 *Write corresponding BVP's related to the above chains of equalities.*

8 Real functional (nonlinear problems)

For the following it is convenient to introduce the notation for the complex innerproduct:

$$\langle z_1, z_2 \rangle := \frac{1}{2} \left[z_1 \overline{z_2} + \overline{z_1} z_2 \right] = \text{Re} \left[z_1 \overline{z_2} \right];$$

note that

$$\text{Im} \left[z_1 \overline{z_2} \right] = \langle z_1, i z_2 \rangle = - \langle i z_1, z_2 \rangle.$$

Up to now we have used the complex valued functional $\int \left[(\nabla u)^2 - k^2 u^2 \right]$ that produces the correct HE for linear materials. The real valued functional $\int \left[|\nabla u|^2 - k^2 |u|^2 \right]$ produces the same Helmholtz equation.

Remark 18 *The fact that both functionals produce the same equation is a mathematical degeneracy from the linearity of the problem: the 'weak formulation' of the HE*

$$\int \left[-\Delta u - k^2 u \right] \cdot v = 0$$

is the first variation of the complex valued functional if $\cdot$ is interpreted as the product of complex numbers, but leads just as well to the real valued functional if $\cdot$ is interpreted as the complex innerproduct defined above.

From a physical point of view, the real valued functional is more 'natural', since it appears from the time averaging for time-harmonic solutions $E(z,t) = u e^{i \omega t} + cc$ of the Lagrangian for the time-dependent Maxwell equations

$$\int dt \int \left[\mu_0 \left(\partial_t D \right)^2 - \left(\nabla E \right)^2 \right]$$

As we have stated in the introduction, to deal with nonlinear materials we have to use the functional

$$\mathcal{L}(u) = \frac{1}{2}\int \left[|\nabla u|^2 - k^2|u|^2 - \frac{1}{2}\gamma|u|^4 \right]$$

in order to get the correct equations. This is seen in the standard way from the first variation: from

$$\delta\mathcal{L}(u;v) = \int \left[\langle \nabla u, \nabla v\rangle - k^2 \langle u, v\rangle - \gamma|u|^2 \langle u, v\rangle \right]$$

and with $\delta\mathcal{L}(u;v) = \int \langle \delta\mathcal{L}(u), v\rangle$ it indeed follows that

$$\delta\mathcal{L}(u) = -\Delta u - k^2 u - \gamma\,|u|^2\,u.$$

(In the following we will usually take $\gamma = 0$ to shorten the formulae.)

The functional $\int \left[|\nabla u|^2 - k^2|u|^2 \right]$ has the characteristic property that it *cannot distinguish between right- and left- traveling waves*; in fact the functional vanishes identically for uni-directional waves in uniform media. This is easily seen by substituting a combination of right and left travelling waves (for subsequent use, calculated on a bounded interval):

$$\left\{ \frac{1}{2}\int_{-\ell}^{0} \left[|\partial_z u|^2 - k_-^2|u|^2 \right] \;\middle|\; u = Ae^{ikz} + re^{-ikz} \right\} = -k_- \,\mathrm{Im}\left[A\bar{r} - A\bar{r}e^{-2ik\ell} \right] =: \mathcal{W}_-(A,r).$$

Hence, indeed, if for instance $r = 0$, the functional vanishes identically for uni-directional waves; besides that, note that the result is symmetric in the amplitudes.
The function does define a 'kind' of value function for the reflection-transmission problem but some precautions have to be taken into account. In fact, the function is equal to the value function, which should be interpreted as a function of the fields at the endpoint-values $u(0) = u_0$ and $u(-\ell) = u_{-\ell}$ with the correct relation between the amplitudes and the endvalues:

$$\mathcal{V}_-(u_0; u_{-\ell}) = \mathcal{W}_-(A,r) \text{ with } A + r = u_0, Ae^{-i\ell k} + re^{i\ell k} = u_{-\ell}.$$

Then in the expression for the reflection trasmission problem (with a similar value function for the half-line at the right)

$$\text{Crit } \left\{ \mathcal{V}_-(u_0; u_{-\ell}) + \frac{1}{2}\int_0^L \left[|\nabla u|^2 - k^2|u|^2 \right] + \mathcal{V}_+(u_L; u_{L+M}) \right\}$$

the correct TIBC's are obtained when the variations with respect to u_0 (and u_L) are taken at fixed $u_{-\ell}$ (and u_{L+M}); then, for instance,

$$\begin{aligned} \langle \delta\mathcal{V}_-(u_0; u_{-\ell}), \delta u_0\rangle &= \langle \delta\mathcal{W}_-(A,r), \delta A\rangle + \langle \delta\mathcal{W}_-(A,r), \delta r\rangle \\ \text{with } \delta u_0 &= \delta A + \delta r, \delta A e^{-i\ell k} + \delta r e^{i\ell k} = 0 \end{aligned}$$

it follows

$$\langle \delta\mathcal{V}_-(u_0; u_{-\ell}), \delta u_0\rangle = \langle ik_-(2A - u_0), \delta u_0\rangle$$

leading with $\langle \delta\mathcal{V}_-(u_0; u_{-\ell}), \delta u_0\rangle - \langle \partial_z u|_{z=0}, \delta u_0\rangle = 0$ to the TIBC

$$\partial_z u = ik_-(2A - u_0) \text{ at } z = 0$$

and similarly $\partial_z u = ik_+ u_L$ at $z = L$, the desired and correct TIBC's.

Remark 19 *Here we had to take care to differentiate with respect to* u_0 *while keeping* $u_{-\ell}$ *fixed. When dealing with value functions defined for functions on infinite domains that decay to zero, this 'end-value' is automatically frozen,and such precautions are satisfied; see the examples for the soliton and the waveguide modes.*

Exercise 20 *Derive a confined formulation, and the BVP with correct BC's, that characterizes the critical frequencies* ω *(if any) for which the inhomogeneity in* $[0, L]$ *is fully transmissive (reflectionless). (Remember that above we used the notation* $k(z) = \omega n(z)$*.) How do you prevent that the solution can be trivial, i.e. prevent that it can be a constant?*

9 2D examples of TIBC's: radiation through a plane

We consider in the uniform plane, $k = k_0$, with horizontal x-axis and vertical z-axis, incoming waves from below ($z < 0$), and want to formulate the x-axis as transmitting boundary or as influx boundary. In all of the following we will use the notation

$$\beta(\ell) = \sqrt{k_0^2 - \ell^2}$$

so that a single plane wave can be written like

$$u = A(\ell)e^{i(\ell x + \beta(\ell)z)}$$

because the wave vector has the correct length $|(\ell, \beta(\ell))|^2 = \ell^2 + \beta^2 = k_0^2$.
A general superposition of plane waves leads to the general solution

$$u = \int A(\ell)e^{i(\ell + \beta z)}d\ell, \text{ for which } \partial_z u = i\int \beta(\ell)A(\ell)e^{i(\ell x + \beta z)}d\ell$$

From this we immediately find the TBC at $x = 0$:

$$\mathcal{D}^+(\psi) = \partial_z u|_{z=0} = iP\psi,$$

where P is a so-called *pseudo-differential operator with symbol* $p(\ell)$ defined by

$$P\psi(x) = \int \beta(\ell)A(\ell)e^{i\ell x}d\ell \text{ for } \psi = \int A(\ell)e^{i\ell x}d\ell$$

Note that this pseudo-differential operator is acting on functions defined on the x-axis: it is a *transversal boundary operator*. This operator is 'global': it cannot be written as a differential operator with only a finite number of x-derivatives.
Some special cases will be considered in the following for which the operator P can be approximated by a finite order transversal differential operator.

9.1 Single plane wave

For a single plane wave $u = Ae^{i(\ell x + \beta(\ell)z)}$ we have

$$u|_{z=0} = Ae^{i\ell x}, \partial_n u = \partial_z u|_{z=0} = iA\beta(\ell)e^{i\ell x}$$

and thus is the DtN-operator (for outgoing single waves)

$$\mathcal{D}^+(\psi) = i\beta(\ell)\psi(x) \text{ for } \psi = Ae^{i\ell x}$$

9.2 Waves near one main direction (diffused light)

Now consider a continuum of wave directions concentrated around a single wave direction: diffused light. We have to distinguish two cases: near-vertical influx. and oblique influx.

9.2.1 Near vertical influx

Approximations for waves that come in almost perpendicular, i.e. mainly in z-direction (ℓ small):

$$\beta(\ell) = \sqrt{k_0^2 - \ell^2} \approx k_0 - \frac{1}{2k_0}\ell^2$$

which leads to

$$P(\psi) \approx k_0\psi + \frac{1}{2k_0}\partial_x^2\psi =: P(0;\psi)$$

Hence the DtN-operator is approximated by a second order differential operator, a 'diffused' operator

$$P(0;\cdot) = k_0 + \frac{1}{2k_0}\partial_x^2.$$

9.2.2 Oblique influx

Approximation near a given wave direction $(\ell_0, \beta_0 = \beta(\ell_0)), \ell_0 \neq 0$, write $\ell = \ell_0 + \lambda$, and use $\beta(\ell) = \sqrt{k_0^2 - \ell^2} = \sqrt{\beta_0^2 - 2\lambda\ell_0} \approx \beta_0 - \frac{\ell_0}{\beta_0}\lambda$ so that

$$\begin{aligned}
P(\psi) &\approx \int \left(\beta_0 - \frac{\ell_0}{\beta_0}\lambda\right) A(\ell_0+\lambda)e^{i(\ell_0+\lambda)x}d\lambda = \\
&= \beta_0\psi - \frac{\ell_0}{\beta_0}\int \lambda A(\ell_0+\lambda)e^{i(\ell_0+\lambda)x}d\lambda = \beta_0\psi - \frac{\ell_0}{\beta_0}\left(-i\partial_x\psi - \ell_0\psi\right) \\
&= \frac{k_0^2}{\beta_0}\psi + i\frac{\ell_0}{\beta_0}\partial_x\psi =: P(\ell_0;\psi)
\end{aligned}$$

Hence the DtN-operator is approximated by a first order differential operator, the 'diffused' operator

$$P(0;\cdot) = \frac{k_0^2}{\beta_0} + i\frac{\ell_0}{\beta_0}\partial_x.$$

9.3 Waves from various directions

9.3.1 Discrete directions

Inflow from two directions:

$$\begin{aligned}
u &= \psi_1 e^{i(\ell_1 x + \beta_1 z)} + \psi_2 e^{i(\ell_2 x + \beta_2 z)}, \\
\mathcal{D}^+(\psi) &= \partial_z u|_{z=0} = iP(\psi)
\end{aligned}$$

with

$$P(\psi) = \beta_1\psi_1 e^{i\ell_1 x} + \beta_2\psi_2 e^{i\ell_2 x}$$

We would like to express the normal derivative in terms of the restriction of the function on the x-axis. This can be done as follows.

$$\begin{pmatrix} \psi \\ \psi_x \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ i\ell_1 & i\ell_2 \end{pmatrix}\begin{pmatrix} \psi_1 e^{i\ell_1 x} \\ \psi_2 e^{i\ell_2 x} \end{pmatrix}$$

$$\begin{aligned}
P(\psi) &= \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \cdot \begin{pmatrix} \psi_1 e^{i\ell_1 x} \\ \psi_2 e^{i\ell_2 x} \end{pmatrix} \\
&= \begin{pmatrix} 1 & 1 \\ i\ell_1 & i\ell_2 \end{pmatrix}^{-*}\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \cdot \begin{pmatrix} \psi \\ \psi_x \end{pmatrix}
\end{aligned}$$

where the matrix has to be inverted and transposed: $(\circ)^{-*}$(NOT Hermitian conjugate).
In detail, the operator is given by

$$P(\psi) = \frac{\ell_2\beta_1 - \ell_1\beta_2}{\ell_2 - \ell_1}\psi - i\frac{\beta_2 - \beta_1}{\ell_2 - \ell_1}\partial_x\psi$$

Recognize in this operator the 'phase velocity' $\frac{\beta_2-\beta_1}{\ell_2-\ell_1}$
Observe that now the DtN-operator is expressed as a first-order differential operator. Note that the directions have to be known in advance!

Exercise 21 *Show that the formula for oblique influx of diffuse light can be obtained from this formula by taking the difference $\ell_2 - \ell_1$ small.*

The generalization to more discrete directions is clear. For 3 directions

$$\begin{pmatrix} \psi \\ \psi_x \\ \psi_{xx} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ i\ell_1 & i\ell_2 & i\ell_3 \\ (i\ell_1)^2 & (i\ell_2)^2 & (i\ell_3)^2 \end{pmatrix} \begin{pmatrix} \psi_1 e^{i\ell_1 x} \\ \psi_2 e^{i\ell_2 x} \\ \psi_3 e^{i\ell_3 x} \end{pmatrix}$$

$$\begin{aligned} P(\psi) &= \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} \begin{pmatrix} \psi_1 e^{i\ell_1 x} \\ \psi_2 e^{i\ell_2 x} \\ \psi_3 e^{i\ell_3 x} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 1 & 1 \\ i\ell_1 & i\ell_2 & i\ell_3 \\ (i\ell_1)^2 & (i\ell_2)^2 & (i\ell_3)^2 \end{pmatrix}^{-*} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} \cdot \begin{pmatrix} \psi \\ \psi_x \\ \psi_{xx} \end{pmatrix} \end{aligned}$$

Now the DtN-operator is expressed as a second order differential operator.

Exercise 22 *Derive the general expression for influx form N oblique directions:*

$$P(\psi) = \sum_{m=0}^{N-1} q_m \left(i\partial_x\right)^m \psi$$

9.3.2 Waves from various diffused directions

In this case we can combine the results above.
For instance, for diffused influx from two oblique directions we get as approximation

$$P(\psi) \approx \begin{pmatrix} 1 & 1 \\ i\ell_1 & i\ell_2 \end{pmatrix}^{-*} \begin{pmatrix} P(\ell_1;\cdot) \\ P(\ell_2;\cdot) \end{pmatrix} \cdot \begin{pmatrix} \psi \\ \psi_x \end{pmatrix}$$

Note the appearance of the 'diffused' operators in this expression, which will increase the order of the differential operator by one. For instance: (CHECK!!!!!)

$$P(\psi) = \left[\frac{\ell_2}{\ell_2 - \ell_1}P(\ell_1;\cdot) - \frac{\ell_1}{\ell_2 - \ell_1}P(\ell_2;\cdot)\right]\psi - i\left[\frac{P(\ell_2;\cdot) - P(\ell_1;\cdot)}{\ell_2 - \ell_1}\right]\partial_x\psi$$

leading to

$$P(\psi) = \left[k_0^2\left(\frac{\ell_2\beta_2 - \ell_1\beta_1}{\left(\ell_2 - \ell_1\right)\beta_1\beta_2}\right)\right]\psi + i\left[\frac{\left(\ell_2\ell_1 + k_0^2\right)\left(\beta_2 - \beta_1\right)}{\left(\ell_2 - \ell_1\right)\beta_1\beta_2}\right]\partial_x\psi + \left[\frac{\ell_2\beta_1 - \ell_1\beta_2}{\left(\ell_2 - \ell_1\right)\beta_1\beta_2}\right]\partial_x^2\psi$$

Exercise 23 *Give a general formula for N directions of oblique, diffused influx.*

9.4 Remark: Transversal and normal boundary operators

In the above approach to TBC's it is essential, in line with the definition of DtN-operator, that this operator is viewed as a tangential operator, derivatives tangential to the boundary, here differential operators in x. The normal derivative is expressed in a tangential operator.
In the literature sometimes different formulations are found that also include higher than the first order normal derivative. Theoretically speaking this is possible, as we shall show, by using the equation in the interior to replace tangential derivatives by normal derivatives. These formulations are problematic: the interpretation is much less clear, and most probably, in any (numerical) approximation, these will lead to unstable (because incompatible) formulations.
The idea is simply to use the equation to replace $\partial_x^2 u$ by $-(k^2+\partial_z^2)u$ in the expression of the DtN; for instance, defining

$$N(u) := -(k^2+\partial_z^2)u$$

an expression for the DtN-operator $\mathcal{D}(\psi) = iP(\psi)$ with

$$P(\psi) = \Sigma_{m=0}\ q_m (i\partial_x)^m \psi$$

can be rewritten, *for solutions of the equation*, like

$$P = \Sigma_{n=0}\ (-1)^n \left\{q_{2n} + iq_{2n+1}\partial_x\right\} N^n(u)|_{z=0}$$

(formally also valid for inhomogeneous media: $k = k(x,z)$). Of course, replacing only a restricted number of tangential derivatives by normal derivatives using the N-operator is also possible. In all these cases we get a mixed transversal-normal operator that is NOT only depending on the value of a function on the boundary. So, although for solutions it is satisfied (trivially from above), this operator will not define a sensible boundary condition for the second order HE in the interior.

10 TIBC in waveguides

Now consider a uniform waveguide in the z-direction and study the TBC at a vertical intersection.
Suppose we have a (complete) set of modes: $\phi_m(x)e^{i\beta_m z}$ with which the general solution (for waves travelling to the right) can be written like

$$u(x,z) = \Sigma_m\ \psi_m \phi_m(x) e^{i\beta_m z}$$

For a TBC at $z=0$ note that

$$\psi(x) = \Sigma_m\ \psi_m\phi_m(x) \text{ and } \mathcal{D}(\psi) := \partial_z u|_{z=0} = iP(\psi) = \Sigma_m\ i\beta_m\psi_m\phi_m(x)$$

For a finite number of modes, we can express the DtN operator in the function ψ and its derivatives explicitly. For that it should be noted that not the first derivative (like in the previous case) but the second order x-derivative can be expressed in the basic modes again:

$$\partial_x^2\phi_m = \gamma_m\phi_m \text{ with } \gamma_m = (\beta_m^2 - k_0^2(x))$$

Then

$$\begin{pmatrix} \psi \\ \psi_{xx} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ \gamma_1 & \gamma_2 \end{pmatrix} \begin{pmatrix} \psi_1\phi_1 \\ \psi_2\phi_2 \end{pmatrix}$$

$$P(\psi) = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \cdot \begin{pmatrix} \psi_1\phi_1 \\ \psi_2\phi_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ \gamma_1 & \gamma_2 \end{pmatrix}^{-*} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \cdot \begin{pmatrix} \psi \\ \psi_{xx} \end{pmatrix}$$

explicitly:

$$P(\psi) = \left[\frac{\beta_1\gamma_2 - \beta_2\gamma_1}{\gamma_2 - \gamma_1}\right]\psi + \left[\frac{\beta_2 - \beta_1}{\gamma_2 - \gamma_1}\right]\partial_x^2\psi.$$

Remark 24 *Observe that, in general, this result only makes sense provided* $\gamma_2 - \gamma_1 = \beta_2^2 - \beta_1^2 \neq 0$*, i.e. in the case of superposition of non-degenerate modes, which is true for uniform wave guides.*

Exercise 25 *Give the expression for the DtN operator in case of a superposition of 3 modes. Can you generalize to superposition of* N *modes (and find* P *as a differential operator of order* $2N$*).*

Exercise 26 *Consider a straight waveguide in the* z*-direction which is homogeneous outside* $[0, L]$*, inhomogeneous in* $[0, L]$*. Consider the case that a single mode is influxed form the left* $z < 0$*, with specified amplitude* A *In* $[0, L]$ *partial reflection and transmittance will occur. Formulate the confined problem on* $[0, L]$ *with TIBC's, and give the confined variational formulation.*
When it is supposed that reflection and transmission is restricted only to a finite number of modes, define the TIBC with explicit transversal differential operators at the boundaries.