Lectures on Mathematical Optics

Part of Lecture Notes for course

Mathematical Aspects of Modern Optics And Its Applications

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Light is basically a wave phenomenon and the characteristic interference dominates the appearance of many phenomena and is the basis for many technological applications.
Mathematical modelling of the penomena is a challenge that was started by scientific giants like Huygens, Newton and Maxwell. The investigations of these models have profited, and are still profiting, from mathematical-physical methods and, on the other hand, stimulated the development of these methods.
This part of the Lecture Notes is written in the spirit of the interplay between

natural phenomena – physics –
– math modelling – analytical & numerical methods.

I hope that the enthusiasm I've felt in the past years of working in this direction in perfect collaboration with Hugo Hoekstra and others is noticeable in these Lecture Notes and in the accompagnying Project-Assignments.

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Contents

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Setting: the Scalar Maxwell Equation

1 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

$$\begin{array}{lcl} \mathbf{E} & : & \text{electric field} \\ \mathbf{H} & : & \text{magnetic field} \end{array}$$

and the variables

$$\begin{array}{lcl} \mathbf{D} & : & \text{dielectric displacement} \\ \mathbf{B} & : & \text{magnetic induction} \end{array}$$

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. In particular, a functional $\mathcal{H}$ of $\mathbf{E}, \mathbf{H}$ can be found such that

$$\mathbf{D} = \delta_{\mathbf{E}} \mathcal{H} \ , \ \ \mathbf{B} = \delta_{\mathbf{H}} \mathcal{H}.$$

  For instance, in vacuum, the constitutive functional $\mathcal{H}$ on a domain Ω reads

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

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

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

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 'electromagnetic' 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, 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'. The equations become

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

and hence

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

which, using vector identity becomes

$$-\omega^2\mu_0\hat{\mathbf{D}} = \Delta\hat{\mathbf{E}} - \boldsymbol{\nabla}\left(div\hat{\mathbf{E}}\right).$$

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

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

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. Furthermore we will consider solutions in which only one component of the **E**-field is non-vanishing (TE-modes); then

$$\mathbf{E} = (0, E_y, 0), \quad \mathbf{H} = (H_x, 0, H_z)$$

Assuming that the polarization has also only its y-component non-vanishing, MME's become

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

which 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:

$$-\omega^2 \mu_0 D = \Delta E.$$

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-direction, a further simplification is obtained: the MME's become

$$\partial_t D_y = \partial_z H_x, \quad \mu_0 \partial_t H_x = \partial_z E_y$$

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 NLS, Introduction

When the Maxwell equations are restricted to depend on one spatial direction only, the z-direction, there result equations for the y-component of the **E**-field and the x-component of the **H**-field; assuming that also the electric polarization has only its y-component non-vanishing, and restricting to non-magnetic materials, the equations can be written as a bi-directional equation like

$$\partial_z \begin{pmatrix} E \\ H \end{pmatrix} = \begin{pmatrix} 0 & \partial_t \\ \partial_t & 0 \end{pmatrix} \begin{pmatrix} D \\ \mu_0 H \end{pmatrix} \tag{1}$$

which can also be written as the second order scalar equation

$$\partial_z^2 E = \mu_0 \partial_t^2 D$$

In the following we consider lossless material with linear dispersion given by $\hat{\varepsilon}_1(\omega)$ and non-dispersive quadratic and/or qubic nonlinearity[1]; then the dielectric displacement is given by

$$D = \varepsilon_o E + \varepsilon_1 * E + \chi_2 E^2 + \chi_3 E^3$$

and can be written as the variational derivative with respect to E of a constitutive functional

$$\mathcal{C}(E) = \int \left[\frac{1}{2} \left(\varepsilon_0 E^2 + \varepsilon_1 * E \cdot E \right) + \frac{1}{3} \chi_2 E^3 + \frac{1}{4} \chi_3 E^4 \right] dt.$$

The linear dispersion relation for modes $e^{i[kz - \omega t]}$ has two solution branches

$$k = \pm K(\omega) \text{ with } K(\omega) \equiv \frac{\omega}{c} R(\omega) \equiv \frac{\omega}{c} \sqrt{1 + \varepsilon_1(\omega)/\varepsilon_0}$$

with $K(\omega)$ real-valued and skew symmetric for real frequencies. Introducing the 'Hamiltonian'

$$\mathcal{H} = \int \left[\frac{1}{2} \left(\varepsilon_0 E^2 + \varepsilon_1 * E \cdot E \right) + \frac{1}{3} \chi_2 E^3 + \frac{1}{4} \chi_3 E^4 + \frac{1}{2} \mu_0 H^2 \right] dt$$

the equations can be written as a Hamiltonian system evolving in z as follows

$$\partial_z \begin{pmatrix} E \\ H \end{pmatrix} = \begin{pmatrix} 0 & \partial_t \\ \partial_t & 0 \end{pmatrix} \begin{pmatrix} \delta_E \mathcal{H} \\ \delta_H \mathcal{H} \end{pmatrix}.$$

Using well established methods from Classical Mechanics and the analogy with wave propagation in fluid dynamics, we will exploit this structure of the equations for two aims: to derive simplified models that describes waves mainly

[1] Actually, the following can be generalised in many ways: higher order dispersion, dispersion in nonlinear terms, higher order non-linearity; only the lossless character is of importance which implies the existence of a constitutive potential for the dielectric displacement. With the same assumption for the magnetic polarization, magnetic properties can be included as well.

propagating in one direction, and the corresponding envelope equation and some methods to study the actual evolution of solutions.
In the next section we briefly describe the uni-directionalization process that leads to an equation for right travelling waves. Then we derive for sharply peaked pulses envelope equations of NLS-type. For the standard NLS (sNLS) we describe its mathematical-physical structure, and rewrite this equation in terms of real amplitude and phase. Then we describe several special solutions, like solitons, and interpret these as coherent structures (relative equilibria of Classical Mechanics). In the final section we give as a famous example of modulational instability, the Benjamin-Feir analysis for instability of constant amplitude solutions.

3 Uni-directional Maxwell equation

To motivate the uni-directionalization, first consider the equations in vacuum. Then the equation

$$\partial_z^2 E - \frac{1}{c^2}\partial_t^2 E \equiv (\partial_z - \frac{1}{c}\partial_t)(\partial_z + \frac{1}{c}\partial_t)E = 0$$

has as general solution superpositions of wave running to the right and left:

$$E = r(t - z/c) + s(t + z/c)$$

For waves running to the right, the simplified equation $(\partial_z + \frac{1}{c}\partial_t)E = 0$ is a uni-directionalization of the bi-directional equation.
For weakly dispersive, non-linear equations, a similar splitting can be made in a good approximation since right travelling waves generate left travelling waves to a limited extent only, in an order determined by the material effects. Following the uni-directionalization process described in detail in Van Groesen & De Jager [5], the result is the following *uni-directional Maxwell equation (uni-ME)*

$$\partial_z E + \frac{1}{c}\partial_t \left[R(i\partial_t)E + \tilde{\chi}_2 E^2 + \tilde{\chi}_3 E^3\right] = 0 \tag{2}$$

where we use the notation $\tilde{\chi}_{2,3} = \chi_{2,3}/2\varepsilon_0$.
The linear part corresponds to the right-travelling branch of the dispersion relation, $k = K(\omega)$, and can be written like $(\partial_z + iK(i\partial_t))\,E = 0$, which should be compared with the bi-directional linear equation which could be written like

$$(\partial_z - iK(i\partial_t))\,(\partial_z + iK(i\partial_t))\,E = 0.$$

The uni-directional equation inherits the Hamiltonian structure of the bi-directional equation, as can be seen by writing

$$\partial_z E = -\frac{1}{c}\partial_t \bar{\mathcal{H}} \quad \text{with } \bar{\mathcal{H}} = \int \left[\frac{1}{2}RE \cdot E + \frac{1}{3}\tilde{\chi}_2 E^3 + \frac{1}{4}\tilde{\chi}_3 E^4\right] dt. \tag{3}$$

The corresponding magnetic field is for this uni-directional propagation given by $H = -\sqrt{\frac{\varepsilon_0}{\mu_0}}E$.

Remark 1 *In the theory of surface waves on a layer of fluid, a similar equation (with z and t interchanged, and for long-wave dispersion approximated by $R = 1 + \partial_t^2$) is known as the Korteweg - de Vries (KdV) equation; it describes uni-directional waves in a remarkably good approximation*[2].

4 Envelope equation for the uni-directional model with χ_3

In this section we will derive the equation for the envelope of a wave group centered at a central frequency $\bar{\omega}$. The result will be, as can be expected, an NLS-type of equation, with coefficients determined by the dispersion relation. The results are simplest to derive and to interpret for qubic nonlinearity, and therefore we will simplify the presentation and only consider the case that $\chi_2 = 0$ and $\chi_3 \neq 0$ and make the following scaling

$$z^* = z/c \text{ and } u = \sqrt{\chi_3}E \tag{4}$$

so that uni-ME becomes (suppressing the asterisk):

$$\partial_z u + \partial_t \left[Ru + u^3 \right] = 0. \tag{5}$$

First investigate the linear equation. The general solution of the linearised equation can be written down as

$$u(z,t) = \int \alpha(\omega) e^{i[K(\omega)z - \omega t]} d\omega$$

where α is the spectral function of the field at $z = 0$. Taking an initial spectrum sharply centered at $\bar{\omega}$, the resulting wave group is a modulation of a harmonic mode, given by

$$u(z,t) = A(z,t)e^{i\bar{\theta}} + cc, \text{ with } \bar{\theta} = K(\bar{\omega})z - \bar{\omega}t$$

where the amplitude that describes the modulation is given by

$$A(z,t) = \int_0^\infty \alpha(\bar{\omega} + \nu) e^{i[(K(\bar{\omega}+\nu) - K(\bar{\omega}))z - \nu t]} d\nu.$$

This complex amplitude satisfies the linear dispersive equation

$$\partial_z A - i \left[K(\bar{\omega} + i\partial_t) - K(\bar{\omega}) \right] A = 0.$$

For the following it will be convenient to eliminate the first order term in the dispersion by introducing a frame moving with the group velocity $1/K'(\bar{\omega})$, i.e. $\tau = t - K'(\bar{\omega})z, \zeta = z$. Then the equation can be rewritten like:

$$\partial_\zeta A - iK_2(i\partial_\tau)A = 0$$

[2] This KdV-equation, derived in 1895, became particularly known in the sixties of the previous century, when it was identified as one of the first 'completely integrable' nonlinear dispersive partial differential equations; later, the NonLinear Schrödinger (NLS)-equation turned out to be possess a similar structure.

where here and in the following we use the notation

$$K_2(\nu) = K(\bar{\omega} + \nu) - K(\bar{\omega}) - K'(\bar{\omega})\nu.$$

To incorporate the nonlinearity in the deformation of the envelope amplitude, a direct perturbation theory in powers of the amplitude is applied. Resonant terms in third order appear that are made to vanish, in order to obtain uniformly valid solutions, by requiring A to satisfy a certain equation. This equation[3] will be called the generalised NLS-equation and denoted by gNLS:

$$\text{gNLS:} \;\; \partial_\zeta A - iK_2(i\partial_\tau)A + i\gamma|A|^2 A = 0.$$

The interaction coefficient γ is found to be $\gamma = -3\bar{\omega}$.
In the envelope equation above, we have retained the full dispersive properties of the problem, just as in the derivation of the uni-ME in the previous section. This may be less relevant for the envelope equation since then, from the start on, the attention is to waves with a sharply peaked spectrum, while uni-ME is valid for waves with a broad spectrum. However, retaining the full dispersion makes it possible to study the influence of truncating the dispersive properties. Indeed, it is custom to expand the dispersion operator to second or third order, i.e.

$$K_2(\nu) \approx \beta_2 \nu^2 + \beta_3 \nu^3$$

where $\beta_2 = \frac{1}{2}K''(\omega), \beta_3 = \frac{1}{6}K'''(\bar{\omega})$, and then A satisfies

$$\text{dNLS:} \;\; \partial_\zeta A + i\beta\partial_\tau^2 A - \beta_3\partial_\tau^3 A + i\gamma|A|^2 A = 0.$$

Taking $\beta_3 = 0$ there results the standard NLS-equation

$$\text{sNLS:} \; \partial_\zeta A + i\beta\partial_\tau^2 A + i\gamma|A|^2 A = 0;$$

performing a simple scaling transforms this equation to the normalised form

$$\partial_\zeta A + i\partial_\tau^2 A + i\text{sign}(\beta\gamma)|A|^2 A = 0.$$

When $\text{sign}(\beta\gamma) = 1$, this is known as self-focussing (converging) NLS, else defocussing (diverging). For anomalous dispersion, i.e. $K''(\bar{\omega}) < 0$, the equation is self-focussing.
These equations are well known in optics and have been studied extensively; see e.g. [1, 7, 8]. For sNLS, the quadratic function K_2 is even, which is not the case when the third order dispersive term β_3 is included; with this additional term, the equation is known as the Dysthe equation (dNLS), and is capable to describe asymmetric perturbations.

[3] For quadratic nonlinearity, the third order resonance appears through interaction of first with second order effects. The interaction coefficient γ is then much more complicated. See [?, ?, ?] for more details.

5 Math-physical structure of sNLS

In the following we will consider for simplicity the sNLS, although most can easily be adapted to dNLS and gNLS.
First we describe the Hamiltonian form of sNLS, and introduce two physically relevant integrals (constants of the motion). To be able to understand the dynamics, which is rather difficult in terms of the complex amplitude A, it is convenient to introduce the real amplitude and phase (like polar-coordinates). The governing amplitude-phase-equations are then derived by performing the transformation in the action principle (which is technically simpler than the alternative to perform the transformation in the equation itself).

5.1 Hamiltonian structure and first integrals

The sNLS has a Hamiltonian structure (as sME and uni-ME from which it has been derived) of the following form:

$$\partial_\zeta A = i\delta H(A), \text{ with } H(A) = \int \left[\beta_2 |A_\tau|^2 - \frac{1}{2}\gamma |A|^4\right] d\tau \tag{6}$$

and, in fact, the equation can be obtained from the canonical action principle:

$$\int d\xi \left[\left[\int -i\bar{A}\partial_\zeta A d\tau\right] - H(A)\right]$$

5.1.1 First integrals, symmetries and conservation laws

1. The following quadratic functional can be interpreted as the **wave energy (wave power)**, and its flow (infinitesimal symmetry) expresses the Gauge invariance of NLS:

$$\begin{aligned} N(A) &= \int |A|^2 d\tau, \\ \text{with flow} &: \partial_\zeta A = i\delta N(A) = iA, \text{ i.e. } A = c.e^{i\zeta} \end{aligned}$$

   The corresponding conservation law is of the form:

$$\partial_\zeta(|A|^2) + \partial_\tau(...) = 0$$

2. Another quadratic functional could be called **Linear momentum** since its flow is translation symmetry:

$$\begin{aligned} L(A) &= \int i\bar{A}\partial_\tau A d\tau, \\ \text{with flow} &: \partial_\zeta A = i\delta L(A) = -\partial_\tau A, \text{ i.e. } A(\zeta,\tau) = A(\zeta-\tau,0) \end{aligned}$$

   Corresponding conservation law:

$$\partial_\zeta(i\bar{A}\partial_t A) + \partial_\tau(...) = 0.$$

5.2 Phase-Amplitude equations

5.2.1 Amplitude, phase and LOCAL wave number and frequency

For a better physical interpretation of the complex amplitude A, one often considers the following transformation (Madelung's transformation, which is actually the same as introducing polar coordinates for complex amplitude) and corresponding definitions:

$$
\begin{aligned}
A &= ae^{i\phi}, \text{ and so } u(z,t) = ae^{i\Phi} + cc + hot = 2a\cos(\Phi) + hot \\
a(\zeta,\tau) &: \text{ real amplitude (envelope), } \geq 0;\ E := a^2 \\
\phi(\zeta,\tau) &: \text{ relative phase,} \\
\Phi(\zeta,\tau) &= k_0 z - \omega_0 t + \phi(\zeta,\tau) \text{ total phase} \\
k(\zeta,\tau) &: \equiv \partial_z \Phi = k_0 + \kappa, \quad \kappa = \partial_z \phi \text{ local wave number} \\
\nu(\zeta,\tau) &: \equiv -\partial_t \Phi = \omega_0 + \nu, \quad \nu = -\partial_t \phi \text{ local frequency}
\end{aligned}
$$

Remark 2 *Be aware:*

1. *even when other coordinates are introduced (ζ,τ), the wave number and frequency have to be defined as derivatives of phase with respect to* physical *variables z, t for a correct physical interpretation. And even then, these notions are not undisputable.*

2. *now κ and ν have nothing to do anymore with variables of Fourier transform!!*

3. *the Madelung's transformation has a different interpretation as complexification of real signal (using Hilbert transform).*

5.2.2 Transformation of VP

To find the equations for a, ϕ from the NLS equation for A, we exploit the canonical action principle. To that end, use $\partial_t \left[f(t)e^{i\phi}\right] = \left[(\partial_t + i\phi_t) \circ f\right] \cdot e^{i\phi}$ for any $f(t)$ and correspondingly for ∂_x.
Then, transformation of action:

$$\int\int -i\bar{A}\partial_\zeta A d\tau d\zeta = \int\int \phi_\xi E d\tau d\zeta$$

and of Hamiltonian

$$
\begin{aligned}
H(a,\phi) &= \int \left[\beta_2 \left[(\partial_\tau a)^2 + \nu^2 a^2\right] - \frac{1}{2}\gamma a^4\right] d\tau \\
&= \int \left[\beta_2 \left[\frac{(\partial_\tau E)^2}{4E} + \nu^2 E\right] - \frac{1}{2}\gamma E^2\right] d\tau
\end{aligned}
$$

5.2.3 Phase-amplitude eqn's

The eqn's now follow immediately from canonical action functional viewed as a functional of ϕ and a (or E) $A(\phi, a)$:

1. *energy equation* from variations with respect to phase $\delta\phi$:

$$\partial_\zeta \left[\frac{\partial A}{\partial \phi_\zeta}\right] + \partial_\tau \left[\frac{\partial A}{\partial \phi_\tau}\right] = 0$$

so

$$\partial_\zeta [E] - \partial_\tau [2\beta_2 \nu E] = 0.$$

This result corresponds to 'energy' conservation in physical variables:

$$\partial_z \left[\frac{\partial A}{\partial \kappa}\right] - \partial_t \left[\frac{\partial A}{\partial \nu}\right] = 0$$

which can be written like

$$\partial_z E + \partial_t [K'(\omega_0 + \nu) \cdot E] = 0, \tag{7}$$

a variant of $\partial_t E + \partial_z (VE) = 0$, with V the groupvelocity.

2. *phase equation* from variations with respect to a (E):

$$\phi_\zeta - \beta_2 \nu^2 + \gamma E + \beta_2 \frac{a_{\tau\tau}}{a} = 0$$

which can be written like a nonlinear dispersion relation (NDR)

$$\text{NDR:} \;\; K(\omega) - k = \gamma E + \beta_2 \frac{a_{tt}}{a} \tag{8}$$

In addition to this equation, one has to remember the definitions of local wave number and frequency, and the resulting kinematic relation

$$\partial_z \omega + \partial_t k = 0 \tag{9}$$

Remark 3 *The* relevance of the phase-amplitude eqn's *is two-fold: a more direct physical interpretation (a describing the 'envelope' of the wave group, ω, k the properties of the carrier wave below the envelope), and an essential means in the analysis of (special) solutions, as we shall see in the next section.*

5.2.4 Integrals

1. From transforming the quadratic wave energy

$$\begin{aligned} N(a) &= \int a^2 d\tau, \\ \partial_\zeta(a^2) - \partial_\tau(2\beta_2 \nu a^2) &= 0 \end{aligned}$$

the energy equation.

2. The linear momentum related to translation symmetry:

$$\begin{aligned} L(a,\phi) &= \int \phi_\tau a^2 d\tau, \\ \partial_\zeta(\nu a^2) - \partial_\tau(P) &= 0, \text{ with } P = 2\beta a_\tau^2 + 2\beta a^2 \phi_\tau^2 - \frac{3}{4}\gamma a^4 \end{aligned}$$

6 Coherent structures: special solutions (nonlinear harmonic, soliton,etc.) of sNLS

NLS combines diverging/converging effects of dispersion and of nonlinearity. When signs are correct, for the 'focussing' NLS, the diverging effect of dispersion, and the confining effect of nonlinearity balance each other and a 'confined' solution like a soliton exist. The converging NLS is most famous for its 1,2, .. N - soliton solutions, which can (accidentally) be written down relatively easy. This is related to the completely integrability of NLS, and the related existence of an infinity of conservation laws (first integrals). We will consider the Self-Focussing/converging NLS in the following.

6.1 Idea of evolution

Consider the amplitude-phase equations. The energy equation and the NDR should be satisfied at each moment and position and together determine the coupled dynamics for ω, k, a. In general, all these quantities change in position and time, but special solutions arise for the case that

$$K(\omega) - k \equiv \mu = \text{constant}. \tag{10}$$

These solutions are physically interpreted as 'coherent structures' (steady states, standing waves). From a mathematical-physical point of view, they can be recognised as the so-called relative equilibria: instead of being equilibria in the usual sense (not changing in ζ and therefore being critical points of the Hamiltonian), a relative equilibrium gives a critical point of the Hamiltonian at a given value of one or more other integrals. With the wave energy and linear momentum taken as integrals for which the value is prescribed, such a relative equilibrium is a constrained critical point, i.e. solution of

$$\text{crit } \{H(A) \,|N(A) = \text{constant},\, L(A) = \text{const}\}\,.$$

Instead of the equation $\delta H(A) = 0$ for a true equilibrium without constraints, the constraints now lead to a modified equation, known as Lagrange's multiplier rule. The result is that a critical point should satisfy for some multipliers the equation

$$\delta\left[(H(A) + \sigma_N N(A) + \sigma_L L(A)\right] = 0.$$

We now consider such solutions.
Basic in the following analysis is the recognition that the NDR can be interpreted in a mechanical analogy as Newtons Law, since it can be written like

$$\beta a_{\tau\tau} - \mu a + \gamma a^3 = 0 \tag{11}$$

where $\mu = K(\omega) - k$. With β the mass of a particle (assumed, or scaled, to be positive), this Newton equation describes the particle motion in a conservative force field with potential P:

$$\boxed{\beta \partial_\tau^2 a = -\frac{\partial}{\partial a} P(a), \text{ potential } P(a) = -\frac{1}{2}\mu a^2 + \frac{1}{4}\gamma a^4} \tag{12}$$

Now, for the special solutions for which μ is constant, this is a simple particle problem and can be analysed with phase plane techniques. The sign of μ and γ will be important for the potential profile. For these solutions the corresponding NLS-amplitude is given by

$$A(\tau,\zeta) = a(\tau)e^{-i\mu\zeta},$$

a pure harmonic modulation $e^{-i\mu\zeta}$ of the fixed profile $a(\tau)$, a 'standing wave'.

Remark 4 *The basic equation (12) can be scaled with a characteristic time T in τ and amplitude q :*

$$a'_{\tau'\tau'} - \mu' a' + p^2 a'^3 = 0, \quad \textit{with } p = \sqrt{\frac{\gamma}{\beta}}qT;$$

μ' can also be scaled to unity (up to sign) by scaling in ζ. Hence, the only fundamental parameter is the parameter p, which indeed plays a special role in the solutions, as can be seen clearly in the case of double pumped pulses (bi-harmonic solutions).

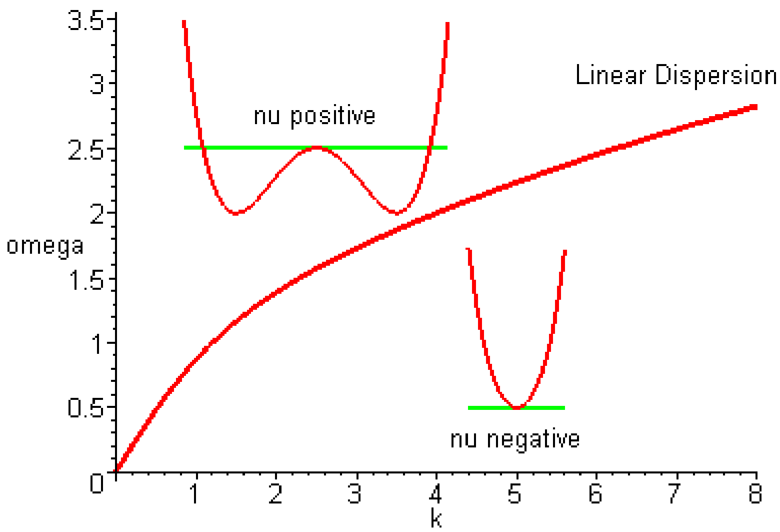
6.1.1 Dispersion plane,Steady soln's, evolution and instability

The dispersion plane (k,ω) is divided in two regions:

K_0	:	the linear dispersion curve (graph) $\{(k,\omega)\,|k = K(\omega)\}$
K^+	:	'above' the linear dispersion curve (epi-graph), $\{(k,\omega)\,|k > K(\omega)\}$
K^-	:	'below' the linear dispersion curve, $\{(k,\omega)\,|k < K(\omega)\}$

Of particular interest are solutions for which k and ω are constant. Then the sign of μ will determine different possibilities. Observe,

$$\text{sign }(\mu) > 0 \text{ in } K^-, \quad \text{sign }(\mu) < 0 \text{ in } K^+$$



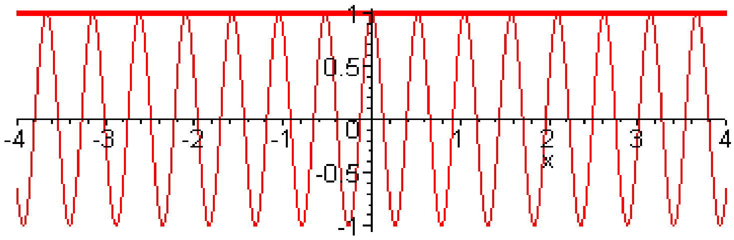
The sign of μ determines the stability of the trivial solution $a \equiv 0$: for $\mu < 0$ the trivial solution is stable, and becomes unstable if μ crosses 0 ('pitch-fork bifurcation') and becomes positive.
Note that for positive μ, the lowest value of the potential is at $a = \pm\sqrt{\frac{\mu}{\gamma}}$, while the potential is negative for $|a| < \sqrt{2}\sqrt{\frac{\mu}{\gamma}}$.
We now describe briefly the various solutions that can exist as is clear from the phase plane analysis.

6.2 Nonlinear harmonic

This is the solution with constant amplitude:

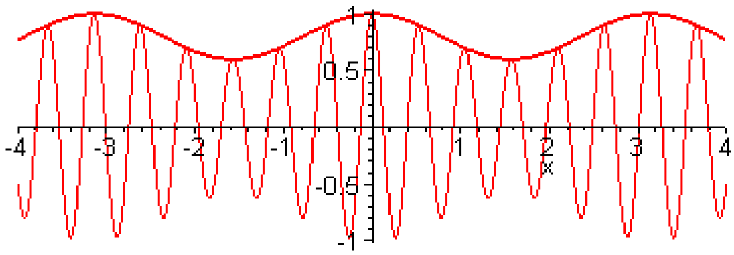
$$A = qe^{-i\gamma q^2 \zeta}$$

which corresponds to the case that $\mu > 0$, and $q = \sqrt{\frac{\mu}{\gamma}}$, is the point of minimal potential. The real part of the NLS-solution is sketched below as function of ζ with the constant amplitude indicated:



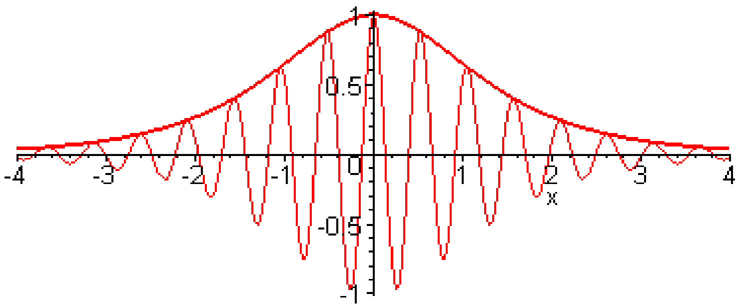
6.3 Nonlinear modulated harmonic

Also for $\mu > 0$, small amplitude periodic motions around the point of minimal potential energy lead to NLS-solutions that are a modulation of the ζ-harmonic:



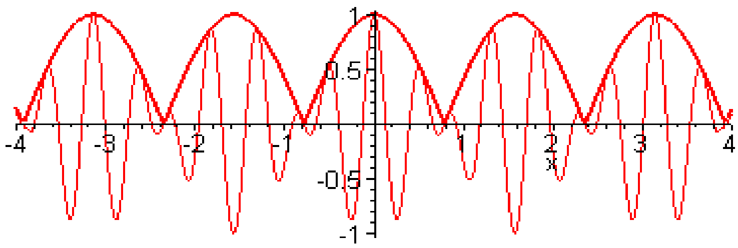
6.4 Soliton

For $\mu > 0$ there exists the famous soliton solution as homoclinic orbit. The amplitude $a = q\mathrm{sech}(q\sqrt{\frac{\gamma}{2\beta}}\tau)$ for $\mu = \gamma q^2/2$ modulates the ζ-harmonic and confines its support:



6.5 Nonlinear bi-harmonic

For $\mu < 0$ the potential is convex, and only periodic solutions can exist that cross the origin. This leads to what could be called 'nonlinear bi-harmonic' solutions:



7 Benjamin-Feir modulational instability

The existence of explicit expressions for solutions as given above does not provide any information about the relevance of such solutions for the total NLS dynamics. Therefore one is usually interested in the stability of these solutions. As illustration of a linear stability analysis we will now show that the nonlinear harmonic (constant amplitude mode) **is linearly unstable**. In fact, the instability is a modulational instability, also called side band instability: there are perturbations which have slightly different wave length (or frequency) that will grow exponentially. This type of instability has first been investigated by Benjamin & Feir.
To investigate the stability, consider small perturbations of the solution:

$$A = q(1+g)e^{-i\gamma q^2 \zeta}$$

where g is a (complex-valued) perturbation. Inserting in NLS, g has to satisfy the linearized eqn:

$$g_\zeta + i\beta g_{\tau\tau} + i\gamma q^2 (g + g^*) = 0.$$

Now investigate the dispersion relation of this equation, which will contain all information. Since there are no real, ζ-dependent solutions, it is handy to substitute

$$g = \left[\alpha_+ e^{i\sigma\tau} + \alpha_- e^{-i\sigma\tau}\right] e^{\rho\xi}$$

and then find for the dispersion relation:

$$\rho^2 + (\beta\sigma^2 - \gamma q^2)^2 = \left[\gamma q^2\right]^2$$

Defining the characteristic 'BF-parameter' p (see also Remark (**??**))

$$p = \frac{q}{\sigma}\sqrt{\frac{\gamma}{\beta}}$$

exponentially growing solution (real $\rho = \rho(\sigma, q)$) exist for $|p| > 1/\sqrt{2}$, i.e. for sufficiently small σ :

$$\rho \text{ is real for } 0 < |\sigma| < \sqrt{2}\sqrt{\frac{\gamma}{\beta}}q$$

The maximal growth factor is

$$\rho = \gamma q^2 \;\; \text{for } p = 1, \text{ i.e. for } \sigma = \pm\sqrt{\frac{\gamma}{\beta}}q$$

Introducing $\frac{\rho}{\gamma q^2} = \sin(2\psi)$, and writing $\alpha_+ = \frac{1}{2}\varepsilon e^{i\psi_0}$, (any ψ_0) the solution can be written like

$$g = \varepsilon e^{\rho\zeta}\cos(\sigma\tau - \psi + \psi_0)e^{i\psi}$$

corresponding to unstable solutions of NLS of the form

$$A = qe^{-i\gamma q^2\zeta}\left[1 + \varepsilon e^{\rho\zeta}e^{i\psi}\cos(\sigma\tau - \psi + \psi_0)\right]$$

Observe the phase shift connected to instability (for maximal growth a shift of $\pi/4$.).

Remark 5 *The **Benjamin-Feir "instability"** of the constant solution shows exponentially growing solutions for* $|\sigma| < \sqrt{2}\sqrt{\frac{\gamma}{\beta}}q$, *i.e. shows LINEAR instability. This doesn't describe how the unstable solution evolves when its value becomes larger. However, and quite remarkably, the full nonlinear solution can be found: it is an* $\tau-$*periodic,* $\zeta-$*soliton solution; the limiting behaviour of this soliton for* $\zeta \to \pm\infty$ *is the exponential growth and decay of the unstable linear expressions found here. See [[1]!*

8 GRATINGS, Introduction

Starting from the scalar Maxwell equation

$$\mu_0 \partial_t^2 D_y = \Delta E_y,$$

we will now restrict to single frequency solutions, i.e. for frequency ω, solutions of the form

$$E_y = u(x,z) e^{-i\omega t} + cc.$$

Then the equation for u becomes:

$$\left[\Delta + \frac{\omega^2 n^2(x,z)}{c^2} \right] u = 0$$

For nonlinear Kerr material, $D_y = \varepsilon_0 \left[n^2 E_y + \chi |E_y|^2 E_y \right]$ with $\chi = \chi_3$ the equation modifies to

$$\left[\Delta + \frac{\omega^2}{c^2} \{ n^2(x,z) + \chi u^2 \} \right] u = 0.$$

Without specifying boundary conditions at this moment, this can formally be seen as an eigenvalue problem for the Laplace operator

$$-\Delta u = \frac{\omega^2}{c^2} \left[n^2(x,z) + \chi u^2 \right] u.$$

The variational structure of the problem can be viewed in two ways, depending on whether ω is given or free. The equation (for given ω) admits the variational principle

$$\int \left[(\nabla u)^2 - \frac{\omega^2}{c^2} (n^2 u^2 + \frac{\chi}{2} u^4) \right],$$

while, when the frequency is to be determined as part of the solution, the eigenvalue problem can also be considered to be the equation for constrained critical points of the variational problem

$$\mathrm{Crit}_u \left\{ \int (\nabla u)^2 \middle| \int (n^2 u^2 + \frac{\chi}{2} u^4) = \text{constant} \right\}$$

with the multiplier interpreted as the squared frequency: $\lambda = \frac{\omega^2}{c^2}$.
In this lecture we will consider devices with nontrivial refractive index variations. In fact we will consider a simple case of a photonic crystal.
A **Photonic crystal** is a material with a periodic index distribution. In such a material PBG's, *Photonic Band Gaps*, may exist: intervals of frequencies for which no propagation of light is possible. Such band gap devices may be used as narrow-band filters, not transmitting all the frequencies inside the gap.

We will study in detail 1 Dimensional problems, so-called *gratings* as an example of a simple 'photonic 1D crystal' to demonstrate the appearance of PBG's. First for a special case that is explicitly solvable, then more general with variational characterization of the PBG.
Standard literature is the book of Joannopoulos et al., [6]; the basic variational methods are treated in many books, and in the Lecture Notes [4].

8.1 Perspective

In the following we consider the simple looking second order differential equation

$$\partial_z^2 u + k^2(z)u = 0$$

where k is given smooth, real function. With z interpreted as time, this is a 'standard' Newton equation, but non-autonomous when k is not constant. Despite it simple appearance, only for very special functions $k(z)$ solutions can be found explicitly. Much research has been, and still is, devoted to understand the behaviour of solutions (like stability) and/or to find approximations. A short overview is as follows.

- For constant $k = \bar{k}$, the equation is the harmonic oscillator with solutions

  $$u = Ae^{i\bar{k}z}$$

  for arbitrary amplitude A; the complex conjugate is also a solution.

- When k varies 'slowly' in z, a first step to find an approximation may be to look for a varying phase, with variations determined by k:

  $$u \approx Ae^{i\theta(z)} \text{ with } \partial_z\theta(z) = k(z).$$

  Variants of this method are the basis of numerical Beam Propagation Methods (BPM).

- The above approximation doesn't satisfy the identity that should hold for each solution (a special case of the conservation of the Poynting vector):

  $$\operatorname{Im} \partial_z \left[u^* \partial_z u\right] = 0.$$

  One can satisfy the Poynting identity by allowing the amplitude to change; then from

  $$\partial_z \left[|A|^2 \partial_z \theta\right] = 0$$

  the following approximation is obtained

  $$u_{WKB}(z) = \frac{A_0}{\sqrt{k(z)}} e^{i\theta(z)} \text{ with } \partial_z\theta(z) = k(z).$$

  This is known as the WKB (Wentzel, Kramer, Brillouin) method; the approximation is remarkably good (asymptotically correct), provided the changes are 'slow' enough.

- Another type of results concern cases when the function k is periodic; for instance periodic changes around a fixed value, so-called Hill's equation,

$$\partial_z^2 u + \left[\bar{k}^2 + \phi(z)\right] u = 0, \quad \phi(z+p) = \phi(p),$$

with Mathieu equation as a special case:

$$\partial_z^2 u + \left[\bar{k}^2 + a\cos(\omega z)\right] u = 0.$$

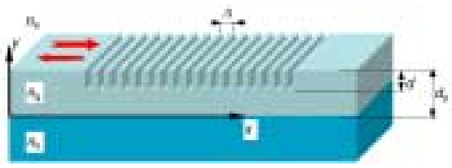
With specialised techniques one analysis the stability of solutions for small a; parametric resonance (instability) appears (for arbitrary small a) when $\bar{k}^2 = (\text{integer} * \omega/2)^2$.

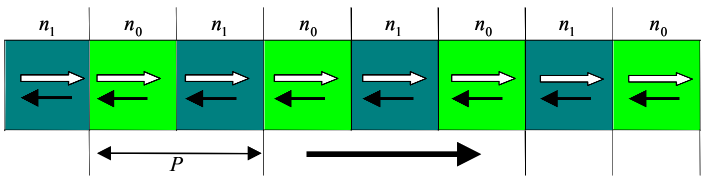
For the periodic structures considered in gratings, $k^2 = \omega^2 n^2$ with n the refractive index, the slowly varying assumption for WKB-methods is not satisfied, and the variations become large, for large frequencies ω. Hence, none of these methods are readily applicable.

9 1D Linear grating: Transfer matrix approach

The standard problem is a material with piecewise constant indices, periodically repeated. For instance,

$$\left[\partial_z^2 + \frac{\omega^2 n^2(z)}{c^2}\right] u = 0\ ,\quad n(z) = \begin{cases} n_0 & \text{for} \quad 0 < z < p/2 \\ n_1 & \text{for} \quad p/2 < z < p \end{cases}$$





This is a nice example since the solution can be found explicitly.

9.1 Period-p Poincaré map

The solution can be written using either real or complex notation. Write, $k_0 = \frac{\omega n_0}{c}$, $k_1 = \frac{\omega n_1}{c}$ and then in successive regions:

$$\begin{aligned} u(z) &= \alpha_0 e^{ik_0 z} + \beta_0 e^{-ik_0 z} = a_0 \cos(k_0 z) + b_0 \sin(k_0 z), \text{ in layer of index } n_0 \\ &= \alpha_1 e^{ik_1 z} + \beta_1 e^{-ik_1 z} \text{ in successive layer of index } n_1 \\ &= \alpha_2 e^{ik_0 z} + \beta_2 e^{-ik_0 z} \text{ in sucessive layer of index } n_0 \end{aligned}$$

Then, conditions of continuity of field & flux through boundaries leads to transfer matrix. (This is a simple example of Coupled Mode Theory.)

Introduce

$$\begin{aligned}\Omega &= \omega p\sqrt{n_0 n_1}/c \\ s &= \frac{k_0+k_1}{2\sqrt{k_0k_1}} = \frac{n_0+n_1}{2\sqrt{n_0n_1}}, v = \frac{n_1-n_0}{2\sqrt{n_0n_1}}; \text{ then } s^2-v^2=1\end{aligned}$$

Observe that s, v are independent of ω, just material properties. The transformation over a full period leads to

$$M = \begin{bmatrix} m_{11} & m_{12} \\ m_{12}^* & m_{11}^* \end{bmatrix}$$

where

$$\begin{aligned}m_{11} &= s^2 e^{i(k_1+k_0)p/2} - v^2 e^{-i(k_0-k_1)p/2} \\ &= \left[s^2\cos s\Omega - v^2\cos v\Omega\right] + i\left[s^2\sin s\Omega + v^2\sin v\Omega\right] \\ m_{12} &= sv\left[e^{i(k_1-k_0)p/2} + e^{-i(k_0+k_1)p/2}\right] \\ &= sv\left[\cos v\Omega + \cos s\Omega\right] + isv\left[\sin v\Omega - \sin s\Omega\right]\end{aligned}$$

Observing $m_{11}^*(\Omega) = m_{11}(-\Omega), m_{12}^*(\Omega) = m_{12}(-\Omega)$, the structure of the map M can be understood:

$$\begin{aligned}\alpha_2 &= m_{11}\alpha_0 + m_{12}\beta_0, \text{ right travelling wave} \\ \beta_2 &= m_{12}^*\alpha_0 + m_{11}^*\beta_0, \text{ left travelling wave}\end{aligned}$$

For real notation: Poincaré map over one period Φ

$$\Phi = RMR^{-1} \text{ with } R = \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}, \Phi = \begin{pmatrix} \text{re}(a+b) & \text{im}(a-b) \\ \text{-im}(a+b) & \text{re}(a-b) \end{pmatrix}$$

9.2 Main property: Volume preserving map

The determinant of the map is the product of its eigenvalues; denoting the eigenvalues by $\lambda_{1,2}$, the determinant is the product of the eigenvalues. In this case the value of the determinant is equal to one:

$$Det = |m_{11}|^2 - |m_{12}|^2 = \left[s^2 - v^2\right]^2 = 1 = \lambda_1 \cdot \lambda_2$$

This could be foreseen since the basic equation is a Hamiltonian system, and hence its flow is area conserving.
Explicitly, the eigenvalues are given by

$$\begin{aligned}\lambda_{1,2} &= r \pm \sqrt{r^2-1} = \cos(\phi) \pm i\sin(\phi), \text{ with } r = \text{Re}(a) = \cos(\phi) \\ r &= s^2\cos s\Omega - v^2\cos v\Omega\end{aligned}$$

Two possibilities:

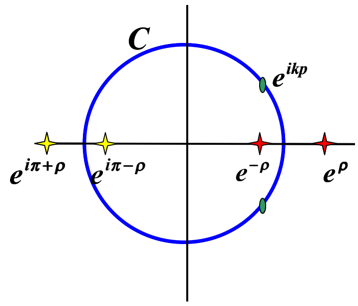
- either both eigenvalues are not real, and then complex conjugate on the unit circle in the complex plane (periodic). We then define the real 'wave number' k by writing

$$\lambda_1 = e^{ikp}$$

This is motivated by writing the eigenvalues like $\lambda_{1,2} = e^{\pm i\phi}$ and interpret ϕ (the so-called Floquet-exponent) as the change in phase over one grating period, so that

$$\phi = k * p, \text{ with } k \text{ the real 'wave number'}$$

- or both eigenvalues are real (exponential solutions),
  - either both positive, and then they an be written like e^{ρ} and $e^{-\rho}$ for some real ρ,
  - or both negative, and then can be written like $e^{i(\pi - i\rho)}$ and $e^{i(\pi + i\rho)}$ for some real ρ



9.3 Photonic Band Gap and Bloch dispersion

We observed that there are no periodic solutions for those values for which eigenvalues are real (not on unit circle). The values for which this is the case define the *Photonic Band Gap.* This is for

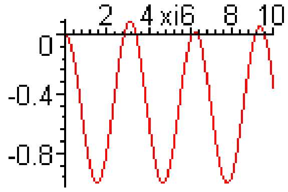
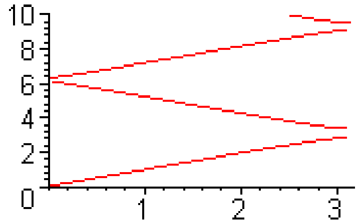
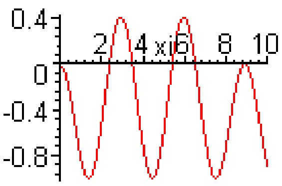
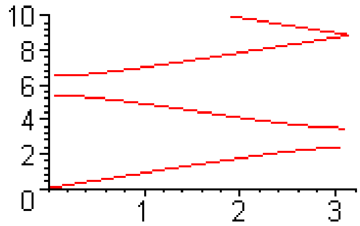
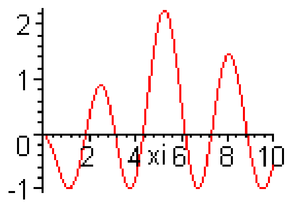
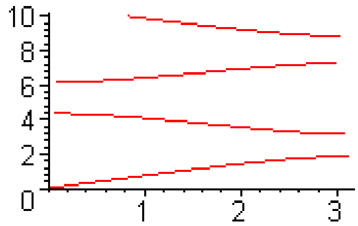
$$PBG: \; r^2 > 1$$

Below we present some pictures, for different index-contrasts; plotted is vertically $r^2 - 1$, horizontally Ω. Outside the PBG the phase ϕ is real, and

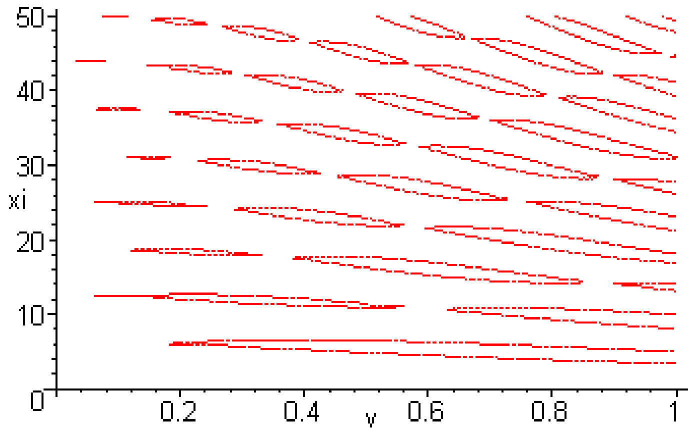
$$\cos(\phi) = \mathrm{Re}(\lambda) = \mathrm{Re}(a) = r, \text{ so } \phi = \arccos(r)$$

Remembering that Ω is a scaled version of the frequency and ϕ of the wave number, the 'dispersion plot' of 'ω vs. k' corresponds to Ω vs. ϕ, shown also in the pictures below. The 'dispersion' found in such gratings is often called Bloch dispersion, to distinguish from dispersion caused by material memory as treated in the first lecture.

Dispersion and PBG plots for given index difference Periodicity makes it possible to restrict the horizontal axis to the interval $[-\pi, \pi]$ (and evenness to $[0, \pi]$).

indices:	PBG: $r^2 - 1 > 0$	dispersion plot
$n_0 = 1.5$ $n_1 = 2$		
$n_0 = 1$ $n_1 = 2$		
$n_0 = 1.5$ $n_1 = 5$		

Plots of Band gap as function of index-difference We can also take the index difference v as variable (horizontally) and Ω vertically, and then plot level sets where $r = 1$ that enclose the areas for PBG. The result is as follows:



9.4 Summary and interpretation

Allowing complex-valued ‘wave numbers’, we can interpret the finding above as characterizing the Bloch dispersion relation

$$k = K(\omega)$$

with different branches as follows:

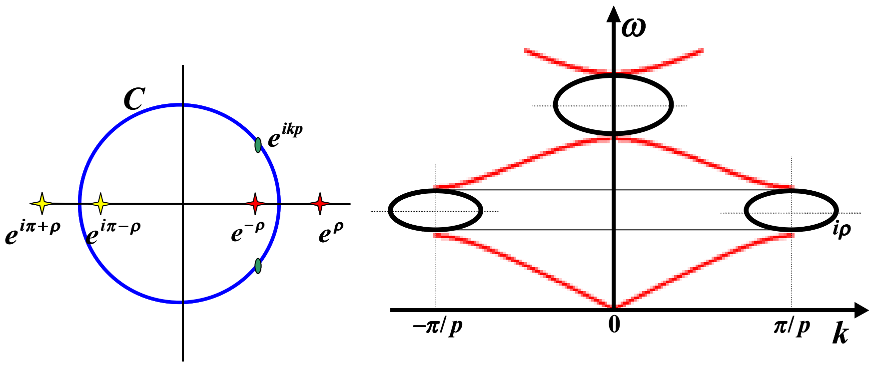
- 'branches' where $k = K(\omega)$ is real for ω outside the PBG; the solutions can be interpreted as travelling waves, $e^{i(kz-\omega t)}$ with phase velocity ω/k;
- the Photonic Band Gaps, for which the complex wave number can be defined as

$$k = K(\omega) = k_g(\omega) \pm i\rho(\omega) \text{ for } \omega \in PBG$$

of two different types:

  - the branches with $k_g = 0$ for which the solutions are periodic with the grating period, harmonic in time and exponentially decreasing/increasing: $e^{\pm\rho z - i\omega t}$ (exponential modulation of standing waves with period p)
  - the branch with $k_g = \pi/p$ for the which the solution looks like $e^{i(z\pi/p-\omega t)}e^{\pm\rho z}$, (the short wave length band-gap, exponential modulation of standing waves with period $2p$).

In one picture, introducing locally imaginary axis in the PBG's, the situation can be sketched as follows:



The Poincaré map provides the information about the evolution of the solution over one grating period. We can associate this with a dynamical system that has the same mapping after one period. This is simplest expressed using the notation above by writing the flow (in z) as

$$\Phi(z) = \begin{pmatrix} e^{iK(\omega)z} & 0 \\ 0 & e^{-iK(\omega)z} \end{pmatrix}$$

such that in a coordinate system of eigenvectors $\Phi(p) = M$. This flow describes the solutions of the corresponding evolution equation in $\mathbf{c} \in C^2$:

$$\partial_z \mathbf{c} = i \begin{pmatrix} K(\omega) & 0 \\ 0 & -K(\omega) \end{pmatrix} \mathbf{c}$$

which is the associated (Hamiltonian) system.

10 Floquet-approach

We will now reconsider the above problem, and at the same time generalize the previous results to periodic index distributions that are not necessarily piecewise constant and for which explicit solutions cannot be written down. The idea is to look at the governing equation as an ODE and use the periodicity of the coefficient to derive special properties.
For non-autonomous ODE's with periodic coefficients,the solutions can be represented in a special way, known as Floquet's Theorem (or Bloch's theorem). We formulate a general result and then the result for the special form of the equation we are interested in.

Theorem 6 ***(Floquet)*** *Consider the first order system of ODE's*

$$\partial_z u + A(z)u = 0$$

where A is a p-periodic matrix: $A(z+p) = A(z)$. Then each solution is of the following form:

$$u(z) = v(z)e^{\rho z}, \quad \textit{with } \rho \in C, \textit{ and } v(z) \textit{ is } P \textit{ -periodic}$$

Note that $u(z+P) = u(z)e^{\rho p}$; the value ρ is called the Floquet exponent, and $e^{\rho p}$ the Floquet multiplier.

Proof. Denote the fundamental matrix solution by $\Phi(z)$. Because of periodicity of $A(z)$, if $u(z)$ is a solution, then so is $u(z+P)$. Hence, there exists a non-singular matrix T such that $\Phi(z+p) = T\Phi(z)$. Since T is non-singular, a matrix B exists such that $T = \exp(Bp)$. Now define $\Psi(z) = \Phi(z)\exp(-Bz)$; then Ψ is p-periodic and Φ is given by

$$\Phi(z) = \Psi(z)\exp(Bz)$$

from which the theorem follows[4]. ∎

Theorem 7 *Consider the second order Hamiltonian system*

$$\partial_z^2 u + q(z)u = 0,$$

where $q(z)$ is a function periodic with period p. Then each solution is of the following form:

$$u(z) = v(z)e^{\pm iKz}, \textit{with } v(z) \textit{ is } p \textit{ -periodic}$$

and with three possibilities (depending on the function q) for the Floquet exponent ρ

- *either $K = k$ is real, and bounded solutions result;*
- *or $K = \pm i\rho$ with ρ real, giving rise to exponential growth multiplying a p-periodic function,*

[4] That is to say, provided the matrix B is (complex) diagonalizable; if B is nil-potent, quasi-exponentials of the form $z^k e^{\rho z}$ arise, with $k = 0, 1, ...$

- *or $K = \pm\pi/p \pm i\rho$ with ρ real, giving rise to exponentially growing solutions multiplying the $2p$-periodic function $v(z)e^{i(z\pi/p)}$.*

Proof. (sketch, without using the result of the general Floquet theorem, but using the basic idea) Motivated by the transfer-matrix method:
Let $u_0(z)$ and $u_1(z)$ be two independent solutions; the linearity makes it possible to express any solution as a linear combination of these two. From the periodicity of q, also $u_0(z+p)$ and $u_1(z+p)$ are solutions, which can therefore be expressed in terms of u_0, u_1, thus defining a transfer matrix T :

$$\begin{pmatrix} u_0 \\ u_1 \end{pmatrix}(z+p) = T \begin{pmatrix} u_0 \\ u_1 \end{pmatrix}(z)$$

The determinant of T is one, as follows from the volume-conservation:

$$\partial_z \left(u_0 \partial_z u_1 - u_1 \partial_z u_1\right)(z) = 0,$$

and hence in particular

$$\left(u_0 \partial_z u_1 - u_1 \partial_z u_1\right)(z+p) = (u_0 \partial_z u_1 - u_1 \partial_z u_1)(z).$$

Then the arguments are as in the previous section. ∎

10.1 Consequences for the grating

Specified for the equation of interest,

$$\left[\partial_z^2 + \omega^2 n^2 (z)\right] u = 0$$

the results have specific consequences.
For $K = \pm i\rho$ the solution is an exponential function $e^{\pm\rho z}$ multiplying a p-periodic function (namely $v(z)$); for $K = \pm\frac{\pi}{p} \pm i\rho$ the solution is an exponential function $e^{\pm\rho z}$ multiplying the function

$$w(z) \equiv v(z)e^{i\pi z/p}$$

This function satisfies

$$w(z+p) = -w(z);$$

in particular, w is $2p$-periodic, but not each $2-$-periodic function satisfies this shift-skew symmetry. For simplicity we will call a functions w that satisfy this condition to be "*p-ss-periodic*".

- We can define the (union of all) PBGaps as

$$\begin{aligned}
\text{PBG} &= \{\omega \,| K(\omega) \text{ is not real}\} \equiv PBG_{+1} \cup PBG_{-1} \\
&= \left\{\omega \,\middle|\, u(z) = v(\omega, z)e^{\pm\rho(\omega)z}, \text{ with } v \text{ is } p\text{-periodic, } \rho \geq 0\right\} \\
&\quad \cup \\
&\quad \left\{\omega \,\middle|\, u(z) = w(\omega, z)e^{\pm\rho(\omega)z}, \text{ with } w \text{ is } p\text{-ss-periodic, } \rho \geq 0\right\}
\end{aligned}$$

The notation $PBG_{\pm 1}$ distinguishes the cases depending on whether the sign of the Floquet multipliers (eigenvalues) is positive or negative.
Observe that the functions v and w inside the PBG satisfy the equation:

$$\partial_z^2 v^\pm \pm 2\rho \partial_z v^\pm + (\omega^2 n^2 + \rho^2) v^\pm = 0, \text{ for } \omega \in PBG$$

together with the (shift-skew-) symmetry condition. Note that solutions with a different index sign are simply related: $v^-(z) = v^+(-z)$.
As one consequence, we can assume the functions v, w to be real, so that these solutions correspond to exponential *standing-waves* for the electric field:

$$\begin{aligned} E &= v(\omega, z) e^{\pm \rho(\omega) z} e^{-i\omega t} \text{ for } \omega \in PBG_{+1} \\ &= w(\omega, z) e^{\pm \rho(\omega) z} e^{-i\omega t} \text{ for } \omega \in PBG_{-1} \end{aligned}$$

Since for $\rho > 0$ the solution will exponentially increase/decrease in the propagation -direction, the light cannot propagate, which is the characteristic property of a PBG.
As we have seen with the transfer-matrix method for a stepwise index structure, we will show later that the PBG consists of infinitely many intervals.

- For $\omega \notin PBG$ we can assume that the real wave numbers belong to the so-called *first Brillouin zone*: $k \in (-\frac{\pi}{p}, \frac{\pi}{p})$ and, from symmetry, actually $k \in (0, \frac{\pi}{p})$. The p-periodic function v satisfies

$$\partial_z^2 v + 2ik \partial_z v + (\omega^2 n^2 - k^2) v = 0, \text{ for } \omega \notin PBG$$

Including the time dependence for the optical field

$$E_y = v(z) e^{ik(\omega) z} e^{-i\omega t},$$

these are travelling wave-like solutions. The relation between frequency and wave number determines the dispersive properties:

$$\text{Bloch dispersion: } \omega \to k(\omega) \in (0, \frac{\pi}{p})$$

- The *boundary of the PBG* is given by the boundary-states:

$$\begin{aligned} \partial \text{PBG} &= \{\omega \,|u(z) = v(\omega, z), \text{ with } v \text{ is } p\text{-periodic}\} \\ & \quad \cup \\ & \quad \{\omega \,|u(z) = w(\omega, z), \text{ with } w \text{ is } p\text{-ss-periodic}\} . \end{aligned}$$

These boundary states satisfy the original equation with additional (shift-skew-) periodicity conditions:

$$\begin{aligned} \partial_z^2 v + \omega^2 n^2 v &= 0, \ v \text{ is } p\text{-periodic, for } \omega \in \partial PBG_{+1} \\ \partial_z^2 w + \omega^2 n^2 w &= 0, \ w \text{ is } p\text{-ss-periodic, for } \omega \in \partial PBG_{-1} \end{aligned}$$

Furtheron we will characterize the values of ω which define the boundaries of the PBG's by characterizing the PBG-boundary-solutions in a variational way.

11 Band gap 'solitons' in nonlinear materials

Now consider propagation in a material with third order nonlinearity

$$\partial_z^2 u + \omega^2 \left[n^2 + \chi |u|^2 \right] u = 0.$$

In a material with constant index n, periodic nonlinear modes exist as generalizations of the linear modes $e^{i\omega n z}$. To see this, refer to the mechanical analogy of a mass particle in a potential $\omega^2 \left[\frac{1}{2} n^2 u^2 + \frac{1}{4} \chi u^4 \right]$, and observe from the phase portrait that all solutions are periodic if $\chi > 0$ and that for $\chi < 0$ the solutions with sufficiently small amplitude are periodic.
For constant index, 'soliton'-type of solutions (decaying at infinity) do not exist since for near vanishing values the solutions will oscillate periodically.
For a grating in this material the situation may be different, since in the absence of nonlinearity the trivial solution $u = 0$ is unstable for $\omega \in PBG$; in fact, inside the PBG a non-smooth function

$$S_{dis} = \begin{cases} v^+ e^{\rho z} \text{ for } z < 0 \\ v^+ e^{\rho z} \text{ for } z > 0 \end{cases}$$

satisfies the correct equation except at $z = 0$. Inclusion of the nonlinearity may allow the corner of S_{dis} to be removed and smoothly connected to form a soliton-type of solution.
To investigate this, we consider a carrier-envelope Ansatz:

$$u = v(z) W(z)$$

where v satisfies the (skew-) periodicity condition of the band gap.
The resulting equation reads

$$W \partial_z^2 v + 2 \partial_z W \partial_z v + v \partial_z^2 W + \omega^2 (n^2 v W + \chi v^3 W^3) = 0.$$

(Note that, indeed, for $\chi = 0$, S_{dis} satisfies this equation outside $z = 0$ for $v = v^{\pm}, W = e^{-\rho|z|}$; for $\chi > 0$ the nonlinearity could possibly compensate a suitable continuisation of the discontinuity).
To apply ideas of 'averaging techniques', the starting point would be the assumption that W varies on a much longer length scale than the function v, which varies on the scale of the grating period. Then multiply the equation by v and integrate over a period, assuming W and its derivatives to be locally constant in such integration interval. The result is

$$\overline{v^2} \partial_z^2 W + \left[\omega^2 \overline{n^2 v^2} - \overline{|\partial_z v|^2} \right] W + \omega^2 \chi \overline{v^4} W^3 = 0$$

Now, taking for $v = v(\omega, z)$ the carrier wave solution in the linear PBG, it holds that

$$\omega^2 \overline{n^2 v^2} - \overline{|\partial_z v|^2} = -\rho^2 \overline{v^2}$$

and hence there results

$$\partial_z^2 W - \rho^2 W + \omega^2 \chi \frac{\overline{v^4}}{\overline{v^2}} W^3 = 0 \tag{13}$$

This averaged envelope equation admits, for $\chi > 0$, standard NLS-type soliton solutions. Such solutions are called *Band Gap Solitons.*

Remark 8 *Observe that the analysis above is not yet a complete proof of the existence of such solitons; technical considerations have to be added for a full proof that the conclusion for this averaged equation carries over for the complete equation. Also, it cannot be excluded that there are also other solutions, such as multi-hump soliton solutions.*

12 Variational characterization of the Band Gaps

Remark 9 *The material in this section seems not to be in the literature and may be new. It is possible to generalise the following to nonlinear materials, and possibly also to 2D (and 3D??) photonic crystals.*

12.1 General outline of the method

We will now find the PBGaps by characterizing the intervals

$$[\omega_{\pm 1}^{m}, \Omega_{\pm 1}^{m}] = PBG_{\pm 1}^{m} \subset PBG_{\pm 1}$$

where ± 1 refers to $\mathrm{PBG}_{\pm 1}$ and $m = 1, 2...$ numbers the successive intervals of increasing ω. We will use the properties of the boundary gap states that were derived in the previous section. These boundary gap states satisfy the original equation

$$\left[\partial_z^2 + \omega^2 n^2(z)\right] u = 0$$

together with some (skew-) symmetry condition. The variational principle

$$\delta \int \left[(\partial_z u)^2 - \omega^2 n^2(z)\, u^2\right] dz = 0$$

leads to the correct equation, but is useless for the present purpose, since the value of ω is unknown and should be sought: our aim is to solve the *eigenvalue problem* which includes the determination of the 'eigenvalue' ω, i.e. we have to deal with free-frequency problem.
Standard methods for linear eigenvalue problems deal with this problem by looking at the critical points of the so-called Rayleigh quotient. An equivalent way (that can be generalised to nonlinear problems) is to study constrained problems. A first formulation is

$$\text{“crit”} \quad \delta \left\{ \int (\partial_z u)^2 dz \,\middle|\, \int \left[n^2(z)\, u^2\right] dz = 1,\ u \in \mathcal{U} \right\} .$$

The set of competing functions in looking for a critical value is implicitly specified by the set $\mathcal{U}$, which includes specification of the boundary or periodicity conditions on the specific interval. If U is a critical point , the Langrange multiplier rule leads to the equation with Lagrange multiplier λ :

$$-\partial_z^2 U = \lambda n^2(z)\, U;$$

by multiplying with U and integration over the interval, anticipating that boundary terms from partial integration will vanish for functions in $\mathcal{U}$, there results

$$\int (\partial_z U)^2 dz = \lambda \int \left[n^2(z)\, U^2\right] dz = \lambda.$$

This shows that the critical value precisely determines the positive multiplier; writing $\lambda = \omega^2$ this produces the desired result:

$$\omega^2 = \text{“crit”} \quad \delta \left\{ \int (\partial_z u)^2 dz \middle| \int \left[n^2(z)\, u^2 \right] dz = 1,\ u \in \mathcal{U} \right\} .$$

Another equivalently formulation can be given that is sometimes easier to deal with; this is actually the ‘inverse’ constrained critical point problem (that has the same solutions but with a different normalization)

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

We will exploit the following orthogonality property for solutions corresponding to different eigenvalues:

$$\begin{aligned} \text{for } -\partial_z^2 U_\lambda &= \lambda n^2(z)\, U_\lambda, \quad -\partial_z^2 U_\mu = \mu n^2(z)\, U_\mu \\ \text{if } \lambda &\neq \mu : \quad \int U_\lambda U_\mu = 0, \quad \int \partial_z U_\lambda \partial_z U_\mu = 0. \end{aligned}$$

A final remark concerns the ‘character’ of the critical point. In the simplest cases (as we shall see, the lowest band gaps), the critical value corresponds to an extremal value and the variational formulation is a constrained maximum or constrained minimum problem. For higher band gaps, the critical point problem will correspond to saddle-point type characterizations (which can be reduced to extremal problems by adding suitable analytic constraints).

12.2 Characterization of PBG$_{-1}$

All boundary states are p-ss-periodic:

$$\partial_z^2 w + \omega^2 n^2 w = 0,\ w \text{ is } p\text{-ss-periodic, for } \omega \in \partial PBG_{-1}.$$

Hence each solution is a shifted odd 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 $p:$ to retain smoothness in the odd continuation, except the vanishing boundary condition, the derivative at begin point and endpoint should be equal but of opposite sign. Since, in general the precise position of the interval is unknown, we also have to find the initial and end point, say ζ and $\zeta + p$. We define the following sets:

$$\mathcal{W}_\zeta = \{ w : [\zeta, \zeta + p] \to IR, |\, w(\zeta) = w(\zeta + p) = 0; \partial_z w(\zeta) = -\partial_z w(\zeta + p) \} ,$$

which is the set of functions that can be continued to p-ss-periodic functions, and the set which satisfy only the Dirichlet conditions:

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

Proposition 10 *For the ‘first’ (lowest) PBG there are two extremal boundary states that determine the gap:*

$$PBG_{-1}^1 = [\omega_{-1}^1, \Omega_{-1}^1]$$

The lowest value ω_{-1}^{1} and the corresponding PBG-boundary state are found from the value (=multiplier) and as the solution of the constrained minimization problem:

$$\left(\omega_{-1}^{1}\right)^{2}=Min_{\zeta,u}\ \left\{\int_{\zeta}^{\zeta+p}\left[(\partial_{z}u)^{2}\right]dz\middle|\int_{\zeta}^{\zeta+p}\left[n^{2}\left(z\right)u^{2}\right]dz=1,u\in\mathcal{W}_{\zeta}^{D}\right\}$$

or equivalently:

$$\left(\frac{1}{\omega_{-}^{1}}\right)^{2}=Max_{\zeta,u}\ \left\{\int_{\zeta}^{\zeta+p}\left[n^{2}\left(z\right)u^{2}\right]dz\middle|\int_{\zeta}^{\zeta+p}\left[(\partial_{z}u)^{2}\right]dz=1,u\in\mathcal{W}_{\zeta}^{D}\right\}$$

Observe that this boundary-solution will have its maximal value at the high-index region.
The upper value Ω_{-1}^{1} and the corresponding boundary state are found by looking for solutions of the following Mini-Max problem:

$$\left(\Omega_{-1}^{1}\right)^{2}=Max_{\eta}\ Min_{u}\ \left\{\int_{\eta}^{\eta+p}\left[(\partial_{z}u)^{2}\right]dz\middle|\int_{\eta}^{\eta+p}\left[n^{2}\left(z\right)u^{2}\right]dz=1,u\in\mathcal{W}_{\eta}^{D}\right\}$$

or equivalently

$$\left(\frac{1}{\Omega_{-1}^{1}}\right)^{2}=Min_{\eta}\ \ Max_{u}\ \left\{\int_{\eta}^{\eta+p}\left[n^{2}\left(z\right)u^{2}\right]dz\middle|\int_{\eta}^{\eta+p}\left[(\partial_{z}u)^{2}\right]dz=1,u\in\mathcal{W}_{\eta}^{D}\right\}.$$

Before proving this proposition, some remarks seem to be in order.

Remark 11

1. *The above variational characterizations are constructive in the sense that they can be used to develop numerical programs: for fixed ζ the function space $\mathcal{W}_{\zeta}^{D}$ can be discretised, then the functionals and then the extremal problem can be solved. Then the extremal values for various values of ζ can be used to determine the optimal value for ζ.*

2. *The special case of a grating with stepwise index that was calculated explicitly before can serve as an example to verify the extremal properties.*

3. *Higher intervals of PBG_{-1} can be found using successive characterizations by restricting the competing functions to satisfy reciprocity conditions with the eigenfunctions of the previous gaps. It may be possible that a few of such 'gaps' are actually 'closed' (see plot in first subsection for $n_0 = 1, n_1 = 2$).*

4. *The normalization in the above characterizations is unimportant since the problem is linear (quadratic functionals). The characterization can be extended to materials with Kerr nonlinearity by using the functional*

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

   instead of $\int_{\zeta}^{\zeta+p}\left[n^{2}\left(z\right)u^{2}\right]dz$. However, now the value of the constraint should be taken into account and the resulting multiplier (and boundary states) will depend on the value of this constraint.

Proof. of the proposition.
Using standard methods from the Calculus of Variations, for fixed interval, a solution U_ζ of the extremizing problems satisfy for a Lagrange multiplier

$$\delta_u \int_\zeta^{\zeta+p} \left[(\partial_z u)^2 - \lambda n^2(z)\, u^2\right] dz = 0$$

i.e.

$$\partial_z^2 U_\zeta = -\lambda n^2 U_\zeta, \quad U_\zeta(\zeta) = U_\zeta(\zeta+p) = 0.$$

Multiplying the equation by U_ζ and integrating over the interval shows that λ is positive and can be associated with $\lambda = \omega^2$.
For the extremal solution on the given interval, the function is sign-definite on the interval, say positive:

$$U_\zeta(z) > 0 \ \text{ for } \ z \in (\zeta, \zeta+p).$$

In general this function will not have the correct conditions for the derivative at the endpoints, i.e. will not belong to $\mathcal{U}_\zeta$. However, by varying the endpoint, say $\zeta \to \zeta + \delta\zeta$ in the functional evaluated at the functions U_ζ, there results

$$\begin{aligned} & \delta_\zeta \int_\zeta^{\zeta+p} \left[(\partial_z U_\zeta)^2 - \lambda n^2(z)\, U_\zeta^2\right] dz \\ = \quad & (\partial_z U_\zeta)^2 - \lambda n^2(z)\, U_\zeta^2 + 2(\partial_z U_\zeta)(\partial_\zeta U_\zeta)\Big|_{z=\zeta}^{z=\zeta+p} = -\left.(\partial_z U_\zeta)^2\right|_{z=\zeta}^{z=\zeta+p}, \end{aligned}$$

the last equality since $U_\zeta(\zeta) = 0$ for each ζ and hence

$$\partial_\zeta U_\zeta(\zeta) = \left[\partial_z U_\zeta(z) + \partial_\zeta U_\zeta(z)\right]_{z=\zeta} = 0,$$

likewise at $z = \zeta + p$. As a consequence, for extremal values, which are achieved by maximizing or minimizing over ζ, at each of these critical values $\bar{\zeta}$ it holds

$$\left.(\partial_z U_{\bar{\zeta}})^2\right|_{z=\bar{\zeta}}^{z=\bar{\zeta}+p} = 0.$$

This shows $\partial_z U_{\bar{\zeta}}(z = \bar{\zeta}) = \pm \partial_z U_{\bar{\zeta}}(z = \bar{\zeta} + p)$. Exploiting the property that $U_{\bar{\zeta}}$ is sign definite, it follows that in fact $\partial_z U_{\bar{\zeta}}(z = \bar{\zeta}) = -\partial_z U_{\bar{\zeta}}(z = \bar{\zeta} + p)$ which shows the required property to be able to extend the solution by shift-skew continuation: $U_{\bar{\zeta}} \in \mathcal{U}_{\bar{\zeta}}$. This finishes the proof of the proposition. ■

12.3 Characterization of PBG$_{+1}$

All PBG$_{+1}$-boundary-states are p-periodic:

$$\partial_z^2 v + \omega^2 n^2 v = 0, \ v \text{ is } p\text{-periodic, for } \omega \in \partial PBG_{+1}.$$

Periodic functions can be found from periodic continuation of functions on the interval

$$\mathcal{V}_{per} = \left\{ v : [\zeta, \zeta+p] \to IR, \,|\, v(\zeta) = v(\zeta+p); \partial_z v(\zeta) = \partial_z v(\zeta+p) \right\};$$

in the variational characterisation below we use the set

$$\mathcal{V} = \{v : [\zeta, \zeta + p] \to IR, | \, v(\zeta) = v(\zeta + p)\} .$$

Actually, the precise choice of the interval is of no relevance in this case, and can be taken arbitrary.
To avoid constant functions v as trivial solution in some of the following variational characterizations, observe that by integrating the equation over one period there results, using periodicity,

$$\int_{period} n^2(z)v(z)dz = 0.$$

(This shows that the solution changes sign in a period, and has vanishing 'average'.)

Proposition 12 *Denote the 'first' (lowest) PBG_{+1} (with $\omega > 0$) by*

$$PBG_{+1} = [\omega^1_{+1}, \Omega^1_{+1}]$$

The lowest value ω^1_{+1} and the corresponding PBG-boundary state are found from the value (=multiplier) and as (a continuation of) the solution of the constrained minimization problem (with the additional natural constraint):

$$\left(\omega^1_{+1}\right)^2 = Min_{u \in \mathcal{V}} \; \left\{ \int_0^p \left[(\partial_z u)^2\right] dz \middle| \int_0^p \left[n^2(z)\, u^2\right] dz = 1, \int_0^p n^2(z)u(z)dz = 0 \right\}$$

or equivalently:

$$\left(\frac{1}{\omega^1_{+1}}\right)^2 = Max_{u \in \mathcal{V}} \; \left\{ \int_0^p \left[n^2(z)\, u^2\right] dz \middle| \int_0^p \left[(\partial_z u)^2\right] dz = 1 \right\}.$$

This boundary-state has its maximal value at the high-index region, and will be denoted by V^{high}_{+1}.
The boundary state corresponding to Ω^1_{+1} is obtained from the same principle in a successive way by restricting to functions 'normal' to V^{high}_{+1}:

$$\left(\Omega^1_{+1}\right)^2 = Min_{u \in \mathcal{V}} \; \left\{ \begin{array}{c} \int_0^p \left[(\partial_z u)^2\right] dz \big| \int_0^p \left[n^2(z)\, u^2\right] dz = 1, \\ \int_0^p n^2(z)u(z)dz = 0, \int_0^p n^2(z)V^{high}_{+1}u(z)dz = 0 \end{array} \right\}$$

or equivalently:

$$\left(\frac{1}{\Omega^1_{+1}}\right)^2 = Max_{u \in \mathcal{V}} \; \left\{ \begin{array}{c} \int_0^p \left[n^2(z)\, u^2\right] dz \big| \int_0^p \left[(\partial_z u)^2\right] dz = 1, \\ \int_0^p n^2(z)V^{high}_{+1}u(z)dz = 0 \end{array} \right\}.$$

Proof. The proof uses standard reasoning from the Calculus of Variations. For the first formulation with the natural constraint, the governing equation contains two Lagrange multipliers and the equation reads

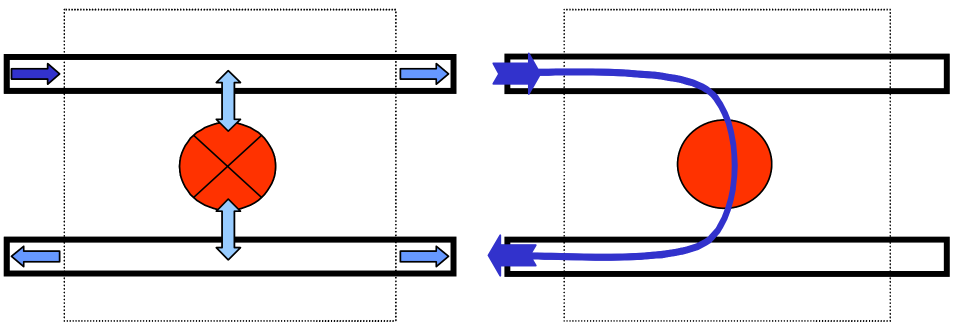
$$\partial_z^2 U + \lambda n^2 U + \sigma n^2 = 0,$$

and the critical point satisfies, in addition to the prescribed boundary condition, the natural boundary conditions: $\partial_z U(0) = \partial_z U(p)$. Integrating the equation, and using the prescribed constraint, shows that $\sigma \int n^2 = 0$, and hence $\sigma = 0$, showing that the critical point satisfies the required equation. This explains the name 'natural' constraint for this functional. An analogous reasoning can be given to show that the constraint $\int_0^p n^2(z)V^{high}_{+1}u(z)dz = 0$ is natural, i.e. doesn't affect the governing equation. ■
Higher PBG's at $k = 0$ can be found using successive characterizations.

Coupling through localised states

13 LOCAL-GLOBAL state coupling, Introduction

Many optical devices (for switching, routing, etc.) consist of input and output waveguides which extent to 'infinity', and another localised component that has the function to route a signal from one of the incoming guides into one of the outgoing guides. To achieve this, the incoming light needs to get a specific influence from local components of the device. The local components determine 'localised states' that influence the global behaviour of the device.
A typical 2D example is a 'micro-resonator' that can act as wavelength filter. It consists of two parallel waveguides with a resonator (ring,or disc) in between that transfers light of one specific wavelength (or, more precisely, from a narrow band of wave lengths) from one waveguide to the other one, and transmits other wavelengths (almost undisturbed) through the same waveguide.
That only specific wavelengths are transferred has as another interpretation and requirement that the local device determines the discrete spectrum of the total device: the eigenmodes of the local component couple only with selective modes of the waveguides.
The general geometric structure of the device is sketched below without specifying the local component.



Transfer and transmittance of light from upper left port; 'generically' output through all ports, 'exceptionally' full transfer (at right).

The general problem is to look for solutions of the Helmholtz equation (we scale such that $c = 1$)

$$\Delta u + \omega^2 n^2 u = 0, \tag{14}$$

where the device is characterised by the refractive index structure $n = n(x, z)$. To be well-posed, specific boundary conditions should be formulated. This is the real problem in optics, which is partly resolved (or obscured) with the idea of light fluxing in and out through certain continua (waveguides).
To make these vague statements more explicit, consider a single waveguide along the z-axis; then for each ω (continuous spectrum), looking for waveguide modes

(satisfying translation symmetry in the z-direction) reduces to the eigenvalue problem for the x-dependent modes ϕ with eigenvalues (the propagation constants) β:

$$u = \phi(x)e^{i\beta z}, \quad \partial_x^2\phi + \omega^2 n^2(x)\phi = \beta^2\phi$$

This leads to a discrete spectrum for β when looking for (x-) decaying modes. From this example it is clear that boundary conditions are essential to determine whether a continuous or discrete spectrum can be expected.
A simpler but comparable case, emphasizing the role of boundary conditions, is the following example.

Example 13 *Role of boundary conditions for the simplest Sturm-Liouville problem. The problem*

$$u_{zz} + \lambda u = 0, \quad u(0) = 0, u(\pi) = 0$$

is the 'standard EVP' with discrete spectrum

$$\psi_k = \sin(kz), \quad \lambda_k = k^2$$

However, for each $\alpha \neq 0$ (the generic case), the problem

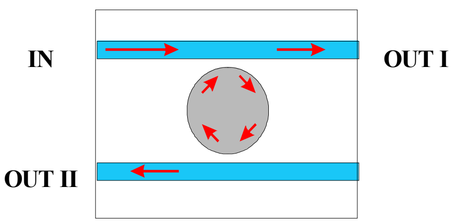
$$u_{zz} + \lambda u = 0, \quad u(0) = 0, u(\pi) = \alpha$$

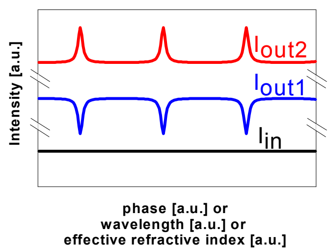
has continuous spectrum,

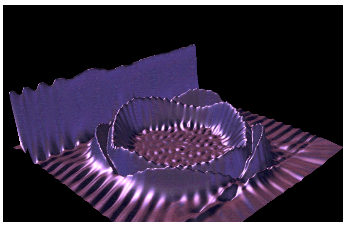
$$\lambda \in IR \backslash \{k^2 | k \in IN\}$$

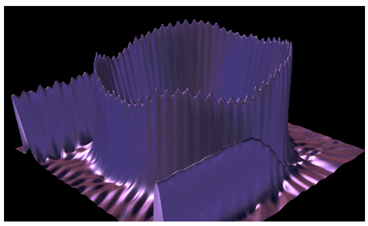
the complement of the above discrete spectrum for the non-generic value $\alpha = 0$.

The same is true, but more difficult to formulate, for the micro-resonator: in-phase states correspond to a discrete spectrum for ω, and out-of-phase to the complement (continuous). This may be 'explained' by first looking at the upper-waveguide: without 'perturbation' of the presence of the resonator, the spectrum is continuous, which (in the generic case) remains to hold when the resonator is present and acts as a perturbation; only exceptionally (non-generic), the spectrum changes. It would be nice to be able to give an explicit characterization for this discrete spectrum. In the following we will consider essentially simplified models to understand this.






Micro-resonator out-of-phase.


Micro-resonator in-phase.

In the following we consider the much simpler analogy of (two) strings coupled to oscillators. This example has been motivated to understand the general formula in [2, 3], and to prepare for treatment of the more difficult optical systems at a later stage. One main lesson to be learned is the importance of symmetry arguments. Different from optical systems, the interaction between the strings is modelled in a simple ad hoc way, while this is one of the most difficult parts for optical devices. Besides this, for the string no radiation is present and one can expect a pure point spectrum for transfer-modes.
For simplicity we first consider a uni-directional model (that 'neglects' reflection) and couple it to an oscillator to see the effect of a point interaction for the transmittance. Then the bi-directional model is investigated which incorporates reflections. Then two parallel strings are studied between which the interaction is determined by the oscillators; then transfer of signals from one to the other string can be studied.

14 Uni-directional string coupled to one oscillator

We first consider the simplest example of a uni-directional equation which has as free solutions waves travelling to the right. At $z = 0$ we introduce a point-coupling to an external force:

$$\partial_t u + c\partial_z u = \alpha r(t)\delta(z).$$

If $r(t)$ is considered as a prescribed function, the forced solution is given by

$$R = \frac{\alpha}{c} r(t - z/c)H(z).$$

Now, instead of externally given, the motion of r is coupled to the free wave. Specifically, as a simple example, a coupling of the string with an oscillator is considered:

$$\dot{r} - i\omega_0 r = -\alpha u(z = 0, t).$$

Then the resulting signal in the string can be written like

$$\begin{array}{rcl} u & = & f + R(f), \\ \text{where} & : & f \text{ is 'free' wave (input)} \\ & : & R(f) \text{ is effect of coupling with local component} \end{array}$$

To demonstrate the effect of the coupling on the transmittance of an incoming wave, we study the two limiting cases of a monochromatic wave and a broad pulse.

14.1 Incoming Monochromatic wave.

Consider the incoming monochromatic free wave

$$f(t - z/c) = Ae^{i\omega^*(t-z/c)}$$

in the string. The oscillator equation becomes

$$\begin{aligned} \dot{r} - i\omega_0 r &= -\alpha \left[f(t) + \alpha r(t)/c \right], \\ \text{i.e.}\quad \dot{r} - (i\omega_0 - \alpha^2/c) r &= -\alpha A e^{i\omega^* t} \end{aligned}$$

with solution

$$r(t) = \frac{i\alpha A}{\omega^* - \omega_0 - i\alpha^2/c} e^{i\omega^* t}.$$

This then leads to the solution in the string of the coupled system

$$\begin{aligned} u(x,t) &= f(t - z/c) + R \\ &= A e^{i\omega^*(t-z/c)} \left\{ \left[1 + \frac{i\alpha^2/c}{\omega^* - \omega_0 - i\alpha^2/c} \right] H(z) + H(-z) \right\} \end{aligned}$$

Conclusion 14 */Interpretation: Coupling with the resonator (oscillator) leads to modification of the original signal; the result can be completely or partly destructive* interference*:*

- when the incoming mode has the same frequency as the oscillator, $\omega_0 = \omega^*$, the incoming monochromatic wave $Ae^{i\omega^*(t-z/c)}H(-z)$ is *completely damped* by destructive interference with the resonator. The presence of the resonator acts like a wall for the incoming wave; since the wave cannot be reflected, its motion is completely transferred to the oscillator motion. This frequency is called the *'resonant' frequency'*.

- for modes of other, non-resonant, frequencies, *partial destruction* takes place; then the incoming wave is 'mildly' attenuated in a Lorentzian-way, i.e. with (tanh-profile) attenuation coefficient:

$$\begin{aligned} \left| 1 + \frac{i\alpha^2/c}{\omega^* - \omega_0 - i\alpha^2/c} \right| &= \left| \frac{\omega^* - \omega_0}{\omega^* - \omega_0 + i\alpha^2/c} \right| \\ &= \frac{\varepsilon}{\sqrt{\varepsilon^2 + 1}} \quad \text{with} \quad \varepsilon = \frac{|\omega - \omega_0|}{\alpha^2/c} \end{aligned}$$

Plot of Lorentzian $\frac{|\varepsilon|}{\sqrt{\varepsilon^2+1}}$

14.2 Incoming pulse.

Now consider the injection of a broad signal. The limiting case is a delta-pulse, i.e. an initial wave $\delta(t-z/c)$. This then leads to an excitement of the resonator

$$\begin{aligned} \dot{r} - i\omega_0 r &= -\alpha\left[\delta(t) + \alpha r/c\right], \\ \text{i.e. } \dot{r} - \left(i\omega_0 - \alpha^2/c\right) r &= -\alpha\delta(t) \end{aligned}$$

with exponentially decaying solution

$$r(t) = \alpha e^{i\omega_0 t} e^{-(\alpha^2/c)t} H(t).$$

For the string the result is an excitement given by

$$R = \frac{\alpha^2}{c} e^{i\omega_0(t-z/c)} e^{-(\alpha^2/c)(t-z/c)} H(t-z/c) H(z);$$

at fixed $z > 0$ the signal decays exponentially in an oscillating way after the signal has arrived at that point, i.e. for $t > z/c$.

Remark 15 *It is a practically important observation that the resulting signal carries the properties of the resonator: by measuring the signal at any position $z > 0$, the coupling constant α and the resonant frequency ω_0 of the oscillator can be found from the decay rate and the oscillating period.*

15 Bi-directional wave equation

Now consider a bi-directional (non-dispersive) wave eqn with two types of forcing:

$$\partial_t^2 u - c^2 \partial_z^2 u = \alpha \dot{r}_e(t)\delta(z) + \beta c r_o(t)\delta'(z).$$

To view the solution as a superposition of waves running in the two directions, note that this equation can also be seen as a system for $u = \frac{1}{2}(U+V)$

$$\begin{aligned} \partial_t U + c\partial_z U &= \delta(z)\left[\alpha r_e(t) + \beta r_o(t)\right] \\ \partial_t V - c\partial_z V &= \delta(z)\left[\alpha r_e(t) - \beta r_o(t)\right] \end{aligned}$$

A consistent coupling to oscillator/resonator is found from variational formulation (Lagrangian):

$$\begin{aligned} &\int\int \left[u_t^2 - c^2 u_z^2\right] dz dt \\ &+ \int \left[\dot{r}_e^2 - \omega_e^2 r^2 + \dot{r}_o^2 - \omega_o^2 r_o^2 + 2\alpha \dot{r}_e u\,(z=0,t) - 2\beta c r_o \partial_z u(z=0,t)\right] dt \end{aligned}$$

leading to the coupled equations:

$$\begin{aligned} u_{tt} - c^2 u_{zz} &= \alpha \dot{r}_e(t)\delta(z) + \beta c r_o(t)\delta'(z) \\ \ddot{r}_e + \omega_e^2 r &= -\alpha\partial_t u(z=0,t) \\ \ddot{r}_o + \omega_o^2 r &= -\beta c \partial_z u(z,t)|_{z=0} \end{aligned}$$

With u interpreted as the vertical deflection, the forcing effect $r_e(t)$ represents forced vertical motion of one point of the string; the forcing $r_o(t)$ can be viewed as twisting (rotating) the string at $z=0$.

Remark 16 *The vertical forcing, and the 'twisting' forcing, can be viewed as the limiting case of equal, respectively opposite, vertical forcing of the string at two different points, say at* $z = -a$*, and* $z = a$ *in the limit* $a \to 0$*.*

15.1 Even mode

Take $\beta = 0$. The forcing $r_e(t)$ leads to waves propagating outward (away from the origin), in equal amounts to the left and the right: the forced solution is an even function in z explicitly given by

$$R_e(z,t) = \frac{\alpha}{2c}\left[r_e(t - z/c)H(z) + r_e(t + z/c)H(-z)\right]$$

With free solution $f(t-z/c)+g(t+z/c)$ the equation for the resonator becomes

$$\begin{aligned} \ddot{r} + \omega_e^2 r &= -\alpha\left[\dot{f} + \dot{g} + \alpha\dot{r}/c\right], \\ \text{i.e. } \ddot{r} + \left(\alpha^2/c\right)\dot{r} + \omega_e^2 r &= -\alpha\left[\dot{f} + \dot{g}\right] \end{aligned}$$

and has solution

$$r_e(t) = \int \frac{i\alpha\omega\left[\hat{f}(\omega) + \hat{g}(\omega)\right]}{-\omega^2 - i(\alpha^2/c)\omega + \omega_e^2} e^{-i\omega t} d\omega$$

Then the total solution becomes

$$\begin{aligned} & u(z,t) \\ = \; & f(t - z/c) + g(t + z/c) \\ & + H(z)\int\left[\frac{1}{2}\frac{i(\alpha^2/c)\omega}{-\omega^2 - i(\alpha^2/c)\omega + \omega_e^2}\right]\left[\hat{f}(\omega) + \hat{g}(\omega)\right] e^{-i\omega(t-z/c)} d\omega \\ & + H(-z)\int\left[\frac{1}{2}\frac{i(\alpha^2/c)\omega}{-\omega^2 - i(\alpha^2/c)\omega + \omega_e^2}\right]\left[\hat{f}(\omega) + \hat{g}(\omega)\right] e^{-i\omega(t+z/c)} d\omega \end{aligned}$$

15.2 Odd mode

Take $\alpha = 0$. The odd mode can be found by differentiating the even mode solution with respect to z. Briefly:
The forcing $r_o(t)$ leads to waves propagating outward (away from the origin), in equal but opposite-signed amounts to the left and the right: the forced solution is an odd function in z explicitly given by

$$R_o(z,t) = \frac{\beta}{2c}\left[-r_o(t - z/c)H(z) + r_o(t + z/c)H(-z)\right]$$

With free solution $f(t - z/c) + g(t + z/c)$ the equation for resonator is

$$\begin{aligned} \ddot{r} + \omega_o^2 r &= -\beta\left[-\dot{f} + \dot{g} + \beta/c\dot{r}\right], \\ \ddot{r} + \beta^2/c\dot{r} + \omega_o^2 r &= -\beta\left[-\dot{f} + \dot{g}\right] \end{aligned}$$

with solution

$$r_o(t) = \int \frac{i\beta\omega\left[-\hat{f}(\omega) + \hat{g}(\omega)\right]}{-\omega^2 - i(\beta^2/c)\omega + \omega_o^2} e^{-i\omega t} d\omega$$

Then the total solution is

$$\begin{aligned}
& u(z,t) \\
= \;& f(t-z/c)+g(t+z/c) \\
& +H(z)\int\left[-\frac{1}{2}\frac{i(\beta^2/c)\omega}{-\omega^2-i(\beta^2/c)\omega+\omega_o^2}\right]\left[-\hat{f}(\omega)+\hat{g}(\omega)\right]e^{-i\omega(t-z/c)}d\omega \\
& +H(-z)\int\left[\frac{1}{2}\frac{i(\beta^2/c)\omega}{-\omega^2-i(\beta^2/c)\omega+\omega_o^2}\right]\left[-\hat{f}(\omega)+\hat{g}(\omega)\right]e^{-i\omega(t+z/c)}d\omega
\end{aligned}$$

15.3 Combined effect of even and odd mode

Combination of the free solution and the forced motions leads to

$$u(z,t)=f(t-z/c)+g(t+z/c)+R_e+R_o.$$

In detail the solution can be written like

$$\begin{aligned}
u(z,t) \;=\;& H(z)*\left[f(t-z/c)+g(t+z/c)+\frac{\alpha}{2c}r_e(t-z/c)-\frac{\beta}{2c}r_o(t-z/c)\right] \\
& +H(-z)*\left[f(t-z/c)+g(t+z/c)+\frac{\alpha}{2c}r_e(t+z/c)+\frac{\beta}{2c}r_o(t+z/c)\right]
\end{aligned}$$

To investigate a specific case, suppose that the free wave consists of an incoming wave at $z=-\infty$ only, i.e. $g=0$. Then

$$\begin{aligned}
u(z,t) \;=\;& H(z)*\left[f(t-z/c)+\frac{\alpha}{2c}r_e(t-z/c)-\frac{\beta}{2c}r_o(t-z/c)\right] \\
& +H(-z)*\left[f(t-z/c)+\frac{\alpha}{2c}r_e(t+z/c)+\frac{\beta}{2c}r_o(t+z/c)\right].
\end{aligned}$$

From this we can conclude that the solution vanishes identically for $z>0$ if we could take for all arguments

$$r_o(s)=-\frac{\alpha}{\beta}r_e(s), \text{ and } \quad r_e(s)=-\frac{c}{\alpha}f(s).$$

This can only be true provided

$$\alpha=\beta, \omega_e=\omega_o.$$

In that case, which special situation is called an *'accidental degeneracy'*, only the single mode signal $f(t)=e^{-i\omega^* t}$ with resonant frequency $\omega^*=\omega_e=\omega_o$, is fully cancelled for $z>0$.

Conclusion 17 *In the case of accidental degeneracy, a mode with resonant frequency coming in from either side, is completely cancelled at* $z=0$.

16 Transfer in coupled strings

It is simple to have the change in the free wave (the effect of R_e and R_o) 'transferred' to another string by taking the same coupling, as shown below.

Denote the deflections of the second string by $v(z,t)$ and assume for simplicity that it has identical properties as the first string. Then from the Lagrangian

$$\int\int \left[u_t^2 - c^2 u_z^2 + v_t^2 - c^2 v_z^2\right] dzdt + \int \left[\dot{r}_e^2 - \omega_e^2 r^2 + \dot{r}_o^2 - \omega_o^2 r_o^2\right] dt +$$
$$\int \left[2\alpha \dot{r}_e \left[u\left(z=0,t\right) - v\left(z=0,t\right)\right] - 2\beta c r_o \left[\partial_z u(z,t) - \partial_z v(z,t)\right]_{z=0}\right] dt$$

one finds the coupled system

$$\begin{aligned}
u_{tt} - c^2 u_{zz} &= \alpha \dot{r}_e(t)\delta(z) + \beta c r_o(t)\delta'(z) \\
\ddot{r}_e + \omega_e^2 r &= -\alpha\partial_t \left[u(z=0,t) - v(z=0,t)\right] \\
\ddot{r}_o + \omega_o^2 r &= -\beta c \partial_z \left[u(z,t) - v(z,t)\right]_{z=0} \\
v_{tt} - c^2 v_{zz} &= -\alpha \dot{r}_e(t)\delta(z) - \beta c r_o(t)\delta'(z)
\end{aligned}$$

With accidental degeneracy, this system is able to completely transfer the mode with resonant frequency.

Remark 18 *By changing the sign of the interactions in the v-string, the transferred mode propagates in the opposite (backward) direction.*

17 Generalization in mode formulation

The above example can be formulated in terms of modes only (replacing the pde by an infinite number of ode's) by using Fourier-expansion in space. Using standard notation, we write

$$u(z,t) = \int u_k(t) e^{ikz} dk, \quad \delta(z) = \int e^{ikz} dk, \delta'(z) = \int ik e^{ikz} dk.$$

Then the string equations become

$$\begin{aligned}
\partial_t^2 u_k + c^2 k^2 u_k &= \alpha \dot{r}_e(t) + ik\beta c r_o(t) \\
\partial_t^2 v_k + c^2 k^2 v_k &= -\alpha \dot{r}_e(t) - ik\beta c r_o(t)
\end{aligned}$$

while the oscillator equations become (note the global coupling to all string modes)

$$\begin{aligned}
\ddot{r}_e + \omega_e^2 r &= -\alpha \partial_t \int \left[u_k(t) - v_k(t)\right] dk \\
\ddot{r}_o + \omega_o^2 r &= -\beta c \partial_t \int ik \left[u_k(t) - v_k(t)\right] dk
\end{aligned}$$

More general systems with Hamiltonian structure for 'mode-oscillator' coupling can be written down. For instance, when the spatial dependence is from waveguide modes, $\psi_k(x,z)$, and the signal in waveguide is given by

$$u(z,t) = \int u_k(t) \psi_k$$

the generalised Fourier-coefficients play the same role as above.

More generally, concentrating on the Hamiltonian structure, the set-up is as follows. In order to guarantee that 'even' and 'odd' modes are possible trough coupling, we consider two local oscillators coupled to 'continua':

$$\begin{aligned} \partial_t u_k &= i\delta_{u_k} H, \quad \partial_t v_k = i\delta_{v_k} H \\ \partial_t r_e &= i\delta_{r_e} H, \quad \partial_t r_o = i\delta_{r_o} H \end{aligned}$$

where H is the Hamiltonian. With the Hamiltonian given in general by

$$\begin{aligned} H(u,v,r) &= \int \left[\frac{1}{2}\omega_1(k)u_k^2 + \frac{1}{2}\omega_2(k)v_k^2 + \frac{1}{2}\omega_e r_e^2 + \frac{1}{2}\omega_o r_o^2 \right] dk \\ &\quad + \int \left[\alpha_e(k)u_k r_e + \alpha_o(k)u_k r_o + \beta_e(k)v_k r_e + \beta_o(k)v_k r_o \right] dk \end{aligned}$$

where interaction coefficients are denoted by α, and $\omega_{1,2}$ describe the properties of the continua, the full equations become

$$\begin{aligned} \partial_t u_k - i\omega_1(k)u_k &= \alpha_e(k)r_e + \alpha_o(k)r_o \\ \partial_t r_e - i\omega_e r_e &= \int \left[\alpha_e(k)u_k + \beta_e(k)v_k \right] \\ \partial_t r_o - i\omega_o r_o &= \int \left[\alpha_o(k)u_k + \beta_o(k)v_k \right] \\ \partial_t v_k - i\omega_2(k)v_k &= \beta_e(k)r_e + \beta_o(k)r_o \end{aligned}$$

Observe that we now have described the complete system as a set of coupled oscillator equations. This formulation allows for easy generalizations, to take into account nonlinearity, additional coupling between the oscillators, etc.