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Theoretical and numerical aspects of Nonlinear Wave Propagation in surface waves and optics

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PREFACE

Wave phenomena in nature, such as in optics and in surface waves, are predominately determined by interference from superposition of various wave components. Dispersion and nonlinearity lead to interesting, often complicated, dynamic evolution of wave patterns.

For understanding the various natural phenomena and for many technological applications, a good description is important. Mathematical models may provide descriptions at various levels, to be used for various purposes.

The basic laws of nature are under certain simplifying physical assumptions well described by sets of partial differential equations for essential physical variables. For fluid dynamics these are the Euler equations, and for electromagnetic fields the Maxwell equations. These equations, although they may provide a valid description, are often far too complicated to be 'understood' in its generality. Modern numerical methods may be exploited to obtain (approximate) solutions. Yet for a further understanding, and to obtain a priori knowledge for the correct design and control of the numerical methods, it is necessary to derive and study simplified models. Such simplified models may be more restrictive (may describe only part of the phenomena, and only approximate) but should have the advantage of being more tractable for theoretical investigations. The derivation of such simplified models can be motivated in various ways, and should actually already indicate information about their domain of validity. In that process of modelling, retaining essential mathematical structures, such as symmetries or variational structures, is essential.

Mathematical modelling of the phenomena is a challenge that was started by scientific giants like Huygens and Newton, and in the 19th century by Maxwell, Scott Russell, Boussinesq, Korteweg & de Vries and many others. In the 20th century, dynamical system theory and improved methods from mathematical physics made it possible to incorporate nonlinear effects to a better extent.

Investigations and simulations of the mathematical models have profited, and are still profiting, from mathematical-physical methods and, on the other hand, stimulated the development of these methods.

These Lecture Notes are written in the spirit of the interplay between

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

Theoretical and numerical aspects of Nonlinear Wave Propagation in surface waves and optics

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Abstract

The lecture notes consist of five sections.

In the first section, basic notions of wave propagation are introduced starting at an elementary level: interference, dispersion, nonlinear effects, and progressing to the description by nonlinear pde's with special mathematical-physical structure.

In sections 2 and 3 the basic 'laws of nature' are given that describe the propagation of light (section 2) and the motion of surface waves (section 3). The most complete description is possible, but too difficult to allow a direct investigation, which motivates the design and study of simplified models, in particular of KdV or NLS-type.

In section 4 some special solutions of the envelope equation, NLS, are considered, and the BF-instability is explained.

Finally in section 5, two basic approaches to numerical methods are described and illustrated: the finite difference method and the finite element method.

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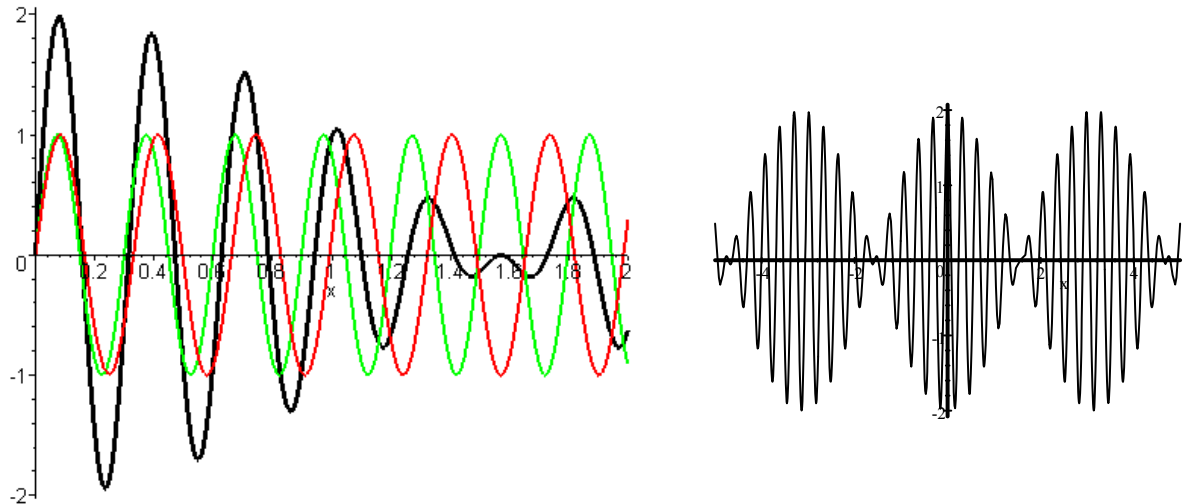
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1 Basic notions Wave Propagation

1.1 Interference

Superposition of 'wiggling' functions can lead to annihilation (cancellation, destructive interference) at some points, and to enlargement (constructive interference) at other points.

For example:



Harmonic function, periodic with period (=wave length)

$$x \rightarrow \cos(kx),$$

$$k \text{ wavenumber, } \lambda = 2\pi/k \text{ wavelength}$$

Superposition of 2 harmonics leads to (harmonic) modulation of harmonic carrier:

$$\cos(k_1x) + \cos(k_2x) = 2 \underbrace{\cos(\Delta kx)}_{\text{modulation}} \underbrace{\cos(\bar{k}x)}_{\text{carrier}},$$

$$\text{with } \Delta k = (k_2 - k_1)/2; \bar{k} = (k_1 + k_2)/2$$

Intermezzo 1 Fourier theory

Any (square integrable) function f can be expressed as a superposition of possibly infinite number of harmonics. With complex notation for Fourier integral:

Provided the 'energy' is finite, i.e.

$$\int_{-\infty}^{\infty} |f(x)|^2 dx < \infty,$$

f can be written like (all integrals over the whole real axis in the following)

$$f(x) = \int F(k) e^{ikx} dk$$

where F , the Fourier-transform of f , is given by

$$F(k) = \frac{1}{2\pi} \int f(x) e^{-ikx} dx.$$

Some basic properties:

1.

$$f \text{ is real, } \Leftrightarrow F(k) = \overline{F(-k)} \quad (\text{overbar is complex conjugate})$$

2.

$$\text{Parseval's identity: } \int |f(x)|^2 dx = \frac{1}{2\pi} \int |F(k)|^2 dk$$

3. and more generally

$$\int f(x)\overline{g(x)}dx = \frac{1}{2\pi} \int \hat{f}(k)\overline{\hat{g}(k)}dk$$

Exercise 2 Show interference ('MAPLE-plot') for bi-harmonic $\cos(14x) + \cos(16x)$.

1.2 Translation wave

Fixed Profile shifted with constant speed:

$$\eta(x,t) = p(x - ct)$$

For harmonic profile, get a harmonic wave:

$$\cos(kx - \omega t)$$

k wave number, ω frequency

ω/k phase velocity

Superposition of two harmonic waves with different phase speed:

$$\cos(k_1x - \omega_1t) + \cos(k_2x - \omega_2t) = 2 \underbrace{\cos(\Delta kx - \Delta\omega t)}_{\text{modulation}} \underbrace{\cos(\bar{k}x - \bar{\omega}t)}_{\text{carrier wave}},$$

lead to a modulation of a carrier wave; both the carrier wave and the modulated wave propagate at their own speed:

$$\text{carrier wave} \quad \cos(\bar{k}x - \bar{\omega}t) \quad \text{speed } \bar{\omega}/\bar{k}$$

$$\text{modulation: amplitude } \cos(\Delta kx - \Delta\omega t), \text{ speed } \Delta\omega/\Delta k \text{ 'group velocity'}$$

Interpretation: superposition of two 'waves', each one propagating with its own phase speed $\frac{\omega}{k}$, leads to 'beat-pattern'.

Animation

Exercise 3 Introduce time dependence and animate ('MAPLE-animate') the bichromatic evolution; verify the propagation speeds of carrier wave and of modulation wave.

1.3 Linear Dispersive wave model

Uni-directional Dispersive wave model: for each wavenumber the physical model assigns a corresponding frequency

$$k \rightarrow \Omega(k),$$

the relation being the so-called *dispersion relation*, such that

$$\exp(i[kx - \Omega(k)t])$$

is a physical solution, a so-called *harmonic 'mode'*.

Example 4 1. *no dispersion: $\Omega(k) = ck$ for some constant c ;*

2. *surface water waves (see next section) in normalised variables:*

$$\text{SW-dispersion: } \Omega(k) = k\sqrt{\frac{\tanh(k)}{k}}$$

and approximated for 'long waves' (i.e. k small)

$$\Omega(k) \approx k(1 - k^2/6)$$

Then Fourier-theory describes the evolution of an initial wave profile:

$$\text{for initial wave profile : } \eta(x, t = 0) = \int \hat{\eta}(k)e^{ikx} dk,$$

$$\text{corresponding evolution : } \eta(x, t) = \int \hat{\eta}(k)e^{i[kx - \Omega(k)t]} dk$$

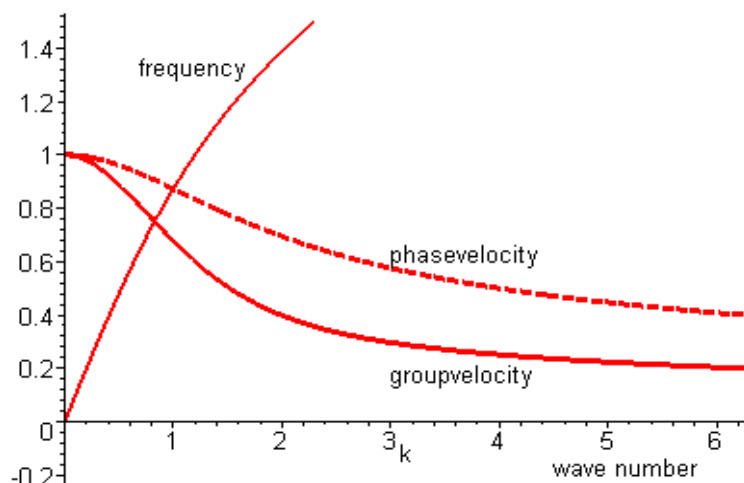
Observe/definition:

1. evolution from real initial data is real, provided $\Omega(k) = -\overline{\Omega(-k)}$
2. evolution is *conservative*, meaning $\int \eta(x, t)^2 dx = \int \eta(x, 0)^2 dx$, provided $\Omega(k)$ is real.
3. The *group velocity* is defined as

$$V_{gr}(k) = \frac{d\Omega(k)}{dk};$$

when there is dispersion, this group velocity is not constant but depends on the wave number.

4. Plot of SW-dispersion, the phase- and groupvelocity:



1.4 Wave groups: modulation

When there is no dispersion, $\Omega(k) = ck$ for some constant c , it is found that

$$\eta(x, t) = \int \hat{\eta}(k) e^{i[kx - \Omega(k)t]} dk = \int \hat{\eta}(k) e^{i[k(x - ct)]} dk = \eta(x - ct, 0),$$

the case of translating wave.

A *monochromatic wave* (complex notation) is obtained for a spectral function that is a delta-function:

$$\hat{\eta}(k) = \delta(k - k_0) \Rightarrow \eta_{monochrom}(x, t) = e^{i[k_0 x - \Omega(k_0)t]}$$

When there is dispersion, the evolution may be much more difficult; a special example is the *bi-chromatic wave* considered above. This example can be rewritten in complex notation with a spectral function consisting of two delta-functions:

$$\hat{\eta}(k) = \delta(k - k_1) + \delta(k - k_2),$$

from which

$$\eta_{bichrom}(x, t) = e^{i[k_1 x - \Omega(k_1)t]} + e^{i[k_2 x - \Omega(k_2)t]}$$

In general, the solution in the form of the Fourier-integral expression is difficult to grasp. However, when the waves have almost the same wavelength, one then talks about a *wave packet*, the evolution can be seen (as in the case of the bichromatic wave) as a modulation of a wave with the main wavelength.

The details of the statement follow from looking at a sharply peaked spectral function, say

$$\hat{\eta}(k) = G(k - k_0)$$

and Taylor expansion of the dispersion relation around $\kappa = k - k_0 \approx 0$:

$$\begin{aligned}\omega(k) &= \Omega_0 + V_0\kappa + \beta\kappa^2 + \dots, \\ \Omega_0 &= \omega(k_0), V_0 = \frac{d\Omega}{dk}(k_0), \beta = \frac{d^2\Omega}{dk^2}(k_0)\end{aligned}$$

Then, the solution can be written as a harmonic wave at the central wavenumber modulated by an amplitude

$$\begin{aligned}\eta(x, t) &= \int G(k - k_0)e^{i[kx - \Omega(k)t]} dk = A(x, t)e^{i[k_0x - \Omega_0t]}, \\ A(x, t) &= \int G(\kappa)e^{i[\kappa(x - V_0t) - \beta\kappa^2t]} dk\end{aligned}$$

Observe that upon neglecting the quadratic terms in the dispersion relation, the amplitude has fixed profile and travels at constant speed V_0 , which is the group velocity at the central wavenumber. For instance, for a Gaussian wave packet,

$$G(\kappa) = \frac{1}{\sigma\pi} \exp[-\kappa^2/(4\sigma^2)]$$

the amplitude is a Gaussian itself:

$$A(x, t) = \exp[-\sigma^2(x - V_0t)^2]$$

In the more general case, the quadratic and higher order terms in the dispersion will lead to some distortion (broadening) of the amplitude's profile. Below we will investigate this deviation by deriving the equation for the amplitude.

1.5 Nonlinearity: mode-interaction and -generation

Most systems, in particular the evolution of surface waves, are non-linear. For instance, in case of Quadratic Nonlinearity, a term appears for which the quantity is squared, say

$$N(\eta) = \eta^2$$

The Fourier transform of a product is not a simple multiplication, but a convolution.

Intermezzo 5 For functions f, g the Fourier transform of the product fg is the convolution of the Fourier-transforms:

$$\widehat{fg}(k) = (\hat{f} * \hat{g})(k) \equiv \int \hat{f}(k - \ell)\hat{g}(\ell)d\ell$$

In the simplest case (verify)

$$e^{i\kappa_1x} \cdot e^{i\kappa_2x} = e^{i(\kappa_1 + \kappa_2)x}$$

which expresses that two Fourier components produce, 'generate', a third one. Clearly, if such nonlinearity is present, modes will be mixed up. For instance, products of long waves produce short waves, and conversely We will see the drastic consequence below.

1.6 Wave Equations: pde's

All the topics above are mathematical methods that are useful to describe phenomena that show characteristic wave properties. But so far no physics (the 'LAWS OF NATURE') has been made explicit. We will discuss this in the next section, but here we just prepare for the general frame work, which is the description by *partial differential equations*. The physical laws, say for the wave elevation $\eta(x, t)$, will be described by relations between the elevation, η , and its derivatives with respect to time $\partial_t \eta$ and space $\partial_x \eta$, and possibly higher order derivatives. (The fact that partial derivatives are involved, explains the name *partial* de, in contrast to *ordinary* de's for functions of only one variable.)

We will now show some examples. As will be relevant for the wave equations, mosttimes we will emphasize the time evolution, that is express $\partial_t \eta$ in terms of the spatial derivatives. This has a fundamental reason: if the equation is of first order in time (meaning that the highest order time derivative is 1, possibly achieved by increasing the number of variables), and some smoothness conditions are satisfied, the IVP (Initial Value Problem) is well posed: for any given initial 'state' (at initial time), the successive evolution (positive time) is uniquely defined.

Translation wave equation

For any profile function p the translation wave: $u(x, t) = p(x - ct)$ satisfies the simple pde

$$\partial_t u = -c \partial_x u$$

and conversely¹!!

Linear Dispersive Wave equation

A single harmonic function $u = \exp(i(kx - \omega t))$ is a special solution (not the only one) of the pde

$$\partial_t u = -\frac{\omega}{k} \partial_x u$$

However, for a dispersive wave model, for which $\omega = \Omega(k)$ is prescribed, this formulation should be generalised as follows. First observe that $\exp(i(kx - \Omega(k)t))$ can be written as a time dependent coefficient multiplying $\exp(ikx)$; writing $a_k(t) = \exp -i\Omega(k)t$, this is for each k a solution of the ode

$$\partial_t a_k = -i\Omega(k)a_k, \quad a_k(0) = 1$$

This motivates to find the equation for the general solution

$$\eta(x, t) = \int \hat{\eta}(k) e^{i[kx - \Omega(k)t]} dk = \int \hat{\eta}(k) e^{-i\Omega(k)t} e^{i[kx]} dk = \int A_k(t) e^{ikx} dk$$

Since

$$\begin{aligned} \partial_t \eta(x, t) &= \int [\partial_t A_k(t)] e^{ikx} dk \\ &= -i \int \Omega(k) \hat{\eta}(k) e^{-i\Omega(k)t} e^{i[kx]} dk = \int [-i\Omega(k) A_k(t)] e^{ikx} dk \end{aligned}$$

¹To show the converse, introduce new variables $\xi = x - ct, v = x + ct$ and observe that the pde becomes in new variables: $\partial_v u = 0$, which is satisfied for any function $u = p(\xi)$, and hence the result.

there results

$$\partial_t A_k = -i\Omega(k)A_k, \quad A_k(0) = \hat{\eta}(k)$$

i.e. each Fourier amplitude satisfies the equation of a simple harmonic oscillator, but with frequency that depends on the wavenumber: $\Omega(k)$.

Intermezzo 6 Pseudo-differential operators

The right hand side is an operator action on the function $\eta(x, t)$ by multiplying each Fourier coefficient of η by $\Omega(k)$ and then inverse Fourier transformation. This so-called Fourier-integral operator, or pseudo-differential operator, will be denoted symbolically as $\check{\Omega}$; it is defined as

$$\text{for } f(x) = \int \hat{f}(k)e^{ikx} dk \quad \text{by definition } \check{\Omega}f(x) = \int \Omega(k)\hat{f}(k)e^{ikx} dk$$

and the function Ω is called the symbol of the operator $\check{\Omega}$.

Example 7 When Ω is a polynomial, the operator $\check{\Omega}$ is a simple differential operator, since

$$\Omega(k) = k, \check{\Omega} = i\partial_x, \quad \text{and hence } \Omega(k) = k^n, \check{\Omega} = (i\partial_x)^n$$

However, $\check{\Omega}$ is also well-defined when it is not a polynomial as in the case of surface waves.

Using this notation, the equation $\partial_t \eta(x, t) = -i \int \Omega(k)A_k(t)e^{ikx} dk$ can be written like

$$\partial_t \eta(x, t) = -i\check{\Omega}\eta(x, t).$$

When $\Omega(k)$ is real (for real k) and odd, this is the general form of a *linear dispersive wave equation*.

Proposition 8 When $\Omega(k)$ is real (for real k) and odd, $\Omega(k) = -\Omega(-k)$, the corresponding pseudo-differential operator is skew-symmetric in the sense that for any two real functions f, g

$$\int f(x)\check{\Omega}g(x)dx = - \int g(x)\check{\Omega}f(x)dx.$$

Proposition 9 For a linear dispersive wave equation the square energy is a constant of the motion:

$$\partial_t \int \eta^2(x, t)dx = 0$$

Exercise 10 Verify (prove) these two propositions.

1.7 Distortion of linear wavegroups: linear envelope equation

Let's now investigate once again the linear wave group, i.e. the solution with a sharply peaked spectral function, say

$$\hat{\eta}(k) = G(k - k_0).$$

From Taylor expansion of the dispersion relation around $\kappa = k - k_0 \approx 0$:

$$\begin{aligned}\omega(k) &= \Omega_0 + V_0\kappa + \beta\kappa^2 + \dots, \\ \Omega_0 &= \omega(k_0), V_0 = \frac{d\Omega}{dk}(k_0), \beta = \frac{d^2\Omega}{dk^2}(k_0)\end{aligned}$$

we found that the solution can be written as a harmonic wave at the central wavenumber modulated by an amplitude

$$\begin{aligned}\eta(x, t) &= A(x, t)e^{i[k_0x - \Omega_0t]}, \\ A(x, t) &= \int G(\kappa)e^{i[\kappa(x - V_0t) - \beta\kappa^2t]}dk\end{aligned}$$

where cubic and higher order terms in the dispersion relation have been neglected.

Using $\xi = x - V_0t$ and $\tau = t$ as the basic variables (which means introducing a frame of reference moving with the group velocity),

$$A(\xi, \tau) = \int G(\kappa)e^{i[\kappa\xi - \beta\kappa^2\tau]}dk$$

Observe that $A(\xi, \tau)$ is the solution of a dispersive wave equation that has dispersion relation $\kappa \rightarrow -\beta\kappa^2$, i.e. A satisfies

$$\partial_\tau A = -i\beta\partial_\xi^2 A.$$

Hence, the distortion of the amplitude of the wavegroup is described by this *envelope equation*. Observe that for $\beta = 0$, the amplitude is fixed, meaning travelling at constant speed V_0 in the laboratory frame of reference.

Exercise 11 Study the 'slow' deformation of the envelope in a wave packet due to dispersion. (Hint: make plots in Maple, subtract the undeformed evolution at the group velocity; approximate the integral by a Riemann sum.)

1.8 Nonlinear wave equation: "Breaking" waves

Consider the following prototype of a nonlinear equation:

$$\partial_t u(x, t) + u(x, t) \partial_x u(x, t) = 0$$

The solution with initial value f can be written analytically in an implicit way as follows. First observe that on a curve $t \rightarrow x(t)$ the total derivative of u is given by

$$\frac{d}{dt} u(x(t), t) = \partial_x u(x(t), t) \frac{d}{dt} x(t) + \partial_t u(x(t), t).$$

From this it follows that

$$\frac{d}{dt} u(x(t), t) = 0 \text{ on } \frac{d}{dt} x(t) = u,$$

and hence

$$u(x, t) = \text{constant on } \frac{d}{dt} x(t) = u.$$

Therefore, the ‘curve’ with $\frac{d}{dt} x(t) = u$, which is called a *characteristic curve*, is in this case a straight line with slope u . From this the construction becomes clear by using the information of the initial value. In detail:

Let y be a point at the x -axis of the x, t plane; at this point u has the value $f(y)$. The characteristic through this point is the straight line with tangent $f(y)$:

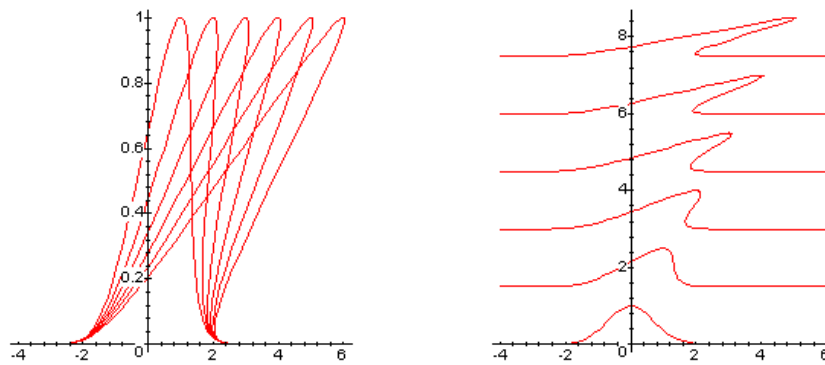
$$x = y + f(y) t$$

and on this line the function u has the value $f(y)$, and so

$$u(y + f(y) t, t) = f(y)$$

is the solution in implicit form.

Example 12 For a Gaussian function as example of an initial profile, the solution can be plotted easily using the parametric representation; a succession of profiles at different times is given below, together with a different presentation that is obtained by shifting the profiles vertically with increasing time.



Exercise 13 Consider the nonlinear “breaking” equation $\partial_t u + u \partial_x u = 0$.

1. Draw the profiles at two successive (positive) times of the solution with initial condition the positive step function:

$$\text{step}(x) = \begin{cases} = 0 & \text{for } x < 0, \\ = 1 & \text{for } x > 0. \end{cases}$$

2. Do the same for the reversed step function, i.e. the initial condition $step(-x)$.
3. Draw in each case characteristic curves in the x, t - plane.
4. Determine the first time t^* at which “breaking” occurs: $\partial_x u(x, t^*) = \infty$.
[[Hint: Note that

$$\frac{d}{dy} u(y + f(y)t, t) = \frac{\partial u}{\partial x}(x, t) \left(1 + t \frac{d}{dy} f(y) \right)$$

and show that from this it follows that on the characteristic through y this is the case for the time (if it exists) such that ..., etc; complete the argument.]]

1.9 Math-physical structure

‘Laws of Nature’ express basic properties and describe special phenomena. Mathematical equations that express these LofN will/should contain these properties and phenomena in the description. That is, such properties will lead to a special structure of the math equations; sometimes this is not obvious, but it is worthwhile to try to *recognise basic properties of physics from the mathematical structure*.

A special example of a basic property is conservation of ‘energy’.

Exercise 14 Show that for the following ode’s in time the given quantity E is conserved (constant in time for solutions)

$$\begin{aligned} \ddot{x} + \omega^2 x &= 0, & E &= \frac{1}{2} (\dot{x}^2 + \omega^2 x^2) \\ \dot{z} + i\omega z &= 0, & E &= \frac{1}{2} |z|^2 \\ \begin{cases} \dot{q} = p \\ \dot{p} = -\omega^2 q \end{cases} & & E &= \frac{1}{2} (p^2 + \omega^2 q^2) \end{aligned}$$

The *phase plane* for these equations is the plane (\dot{x}, x) , $(\text{Re } z, \text{Im } z)$, (q, p) respectively. Level sets of the function E give information about the dynamics (why?). Draw th so-called *phase portrait*, i.e. various levellines in the phase-plane.

These examples are special cases of certain classes of equations, each of which has ‘energy conservation’:

1. Newton’s equation with conservative force from potential energy $V = V(x)$:

$$\ddot{x} + \frac{\partial V}{\partial x} = 0, \quad E = \frac{1}{2} \dot{x}^2 + V(x)$$

2. In complex notation

$$\dot{z} = -i \frac{\partial H}{\partial z}, \quad E = H(z)$$

3. Classical Hamilton's equations in so-called *canonical-variables* (q, p) :

$$\partial_t \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \partial_q H \\ \partial_p H \end{pmatrix}, \quad E = H(q, p)$$

Actually, all these classes of equations themselves are just representatives of one larger class of equations, namely all these are examples of ode's with a Hamiltonian (Poisson) structure.

Definition 15 A dynamical system in R^n (or C^n) with state variable $u(t)$ is called a *Hamiltonian (Poisson) system* if the system of ode's has the following form:

$$\partial_t u = \Gamma \partial_u H(u),$$

where

Γ is a skew-symmetric operator, the 'structure map'

meaning that in a suitable innerproduct

$$\langle \Gamma u, v \rangle = - \langle u, \Gamma v \rangle,$$

and where

$u \rightarrow H(u)$ is a given function, called the Hamiltonian

Exercise 16 Show that the given equations above are indeed Hamiltonian systems by specifying the structure map and the Hamiltonian.

Exercise 17 Show that for a Hamiltonian system the Hamiltonian is a constant of the motion itself:

$$\partial_t H(u) = 0 \text{ for solutions.}$$

Remark 18 This is an example of the opening sentences of this subsection: the mathematical structure of Hamilton's equations implies that there is a constant of the motion (H), i.e. a Hamiltonian structure contains a conservation property.

In Classical Mechanics Hamilton's equations are studied in detail; in most cases the Hamiltonian is (related to) the *total physical energy, sum of kinetic and potential energy*, just as in the examples above.

For systems described by partial differential equations, it is possible to generalise the notion of Hamiltonian system. For instance, all wave equations, when viscous effects which cause dissipation are neglected, can be recognised as such. As a simple example, the translation equation at constant speed

$$\partial_t u = -\partial_x (cu)$$

is of this form:

- the state variable $t \rightarrow u(t)$ now depends on x , i.e. $u(t)(x) = u(x, t)$, and hence $u(t)$ now belongs to an infinite dimensional state space

- the symplectic structure is now

$$\Gamma = \partial_x$$

and is indeed skew-symmetric for the usual L_2 -innerproduct of functions of x that decay at infinity::

$$\langle u, v \rangle = \int u(x)v(x)dx;$$

- the Hamiltonian is now a function on the function space, called functional, in this case given by

$$H(u) = \int \frac{1}{2}cu^2(x)dx;$$

it can be shown that the 'derivative' of such a functional $H(u)$, called the 'variational derivative' and denoted by $\delta H(u)$, can be defined just as for functions on R^n with the directional derivative as a generalisation of the gradient:

$$\langle \delta H(u), v \rangle = \left. \frac{d}{d\varepsilon} H(u + \varepsilon v) \right|_{\varepsilon=0};$$

for the given Hamiltonian

$$H(u) = \int \frac{1}{2}cu^2(x)dx \implies \delta H(u) = cu$$

from which the Hamiltonian structure of the translation equation follows.

Exercise 19 Verify by direct calculation that this Hamiltonian is conserved for solutions of the translation equation (restrict to functions that vanish at infinity). Give also a more direct argument for this result, based on the observation of the change of this functional when the function is translated over an arbitrary distance.

2 Optics

2.1 Macroscopic Maxwell Equations

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

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

where the basic electromagnetic fields are

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

and the variables

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

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_0 constant ($\varepsilon_0 \mu_0 = \frac{1}{c^2}$ 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

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

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:

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

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 ‘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, 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

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

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

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

Applying Gauss’ 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:

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

2.2 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 \mathbf{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):

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

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

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

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

$$\text{Im}(\hat{E}_y \Delta \hat{E}_y^*) = 0$$

2.3 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

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

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

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

2.4 Bi-directional equation

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 \mathbf{E} -field and the x -component of the \mathbf{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

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

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 cubic nonlinearity²; then the dielectric displacement is given by

$$D = \varepsilon_0 E + \varepsilon_1 * E + \chi_2 E^2 + \chi_3 E^3$$

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

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

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’

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

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 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.

² 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.

2.5 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 [4], the result is the following *uni-directional Maxwell equation (uni-ME)*

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

where we use the notation $\tilde{\chi}_{2,3} = \chi_{2,3}/2\epsilon_0$.

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

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

The corresponding magnetic field is for this uni-directional propagation given by $H = -\sqrt{\frac{\epsilon_0}{\mu_0}} E$.

Remark 20 *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 approximation³.*

³This 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.

2.6 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 cubic 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

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

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

$$\partial_z u + \partial_t [Ru + u^3] = 0. \quad (5)$$

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

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

This complex amplitude satisfies the linear dispersive equation

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

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:

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

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 equation⁴ 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, 8, 9]. 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.

⁴For 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.

3 Free Surface Wave Models

The evolution of waves on the surface of a layer of fluid (such as water) remains a challenging task. Assuming the fluid to be incompressible and inviscid, and the flow to be irrotational, the full surface wave equations (full SWE) are well known. The combination of dispersive and non-linear effects present major problems in the numerical simulation as well as in the theoretical analysis of the resulting interesting phenomena.

Although the full SWE's are well known and describe the complete physics, this set of equations is too complicated for a direct investigation. Therefore, to gain insight in interesting characteristic phenomena, except from detailed experiments and numerical simulations, simplified models are desired that are amenable for theoretical investigations, while, at the same time, should be accurate enough to capture the phenomenon of interest.

In this section we present a unified view on results from the literature and describe models of KdV- and NLS-type of equations and their relation. However, since this is essential for the phenomena to be expected, we will carefully model the dispersive properties. That is, we distinguish between long waves (shallow water) and short waves (deep water). In the first case, the dispersion for long waves leads to the classical KdV-equation, and to the defocusing NLS-equation for wave packets. For waves with small wave lengths, comparable to the depth of the fluid, the full dispersive properties should be dealt with, which leads to a non-local version of the KdV-equation and the focusing NLS-equation. In the latter case, initially smooth wave packets will show large deformations (caused by side band instabilities, though different from the well known Benjamin-Feir instability). Using the available results from experiments and simulations, we investigate the performance of the simplified NLS-model.

The mathematical models to be presented, describe, to varying degree of accuracy, the surface wave problem. In all cases, the basic assumptions are that the fluid is incompressible and inviscid (such as water in a good approximation), and that the flow is irrotational; furthermore we mainly restrict to wave propagation in one horizontal direction. The full set of equations (SWE's) is given first. These equations describe in detail the evolution of the surface elevation, and the interior fluid velocity. For designing simpler models, it is important to identify some fundamental properties, which are physically most relevant, and then keep these properties in simplified models. Mass conservation and energy conservation are the most important properties to be retained. Mathematically, the variational structure present in the equations, is just as important to be retained; this is a Hamiltonian structure as briefly discussed in the previous section. The simplified models will be checked for such properties.

A class of simplified models are KdV type of equations for uni-directional wave propagation; these will be considered both for shallow and deep water waves. Finally, for wave packets with narrow banded spectra, NLS-type of equations are described, and the derivation is recalled as far as necessary for the appreciation of the two different cases (focusing and defocusing).

3.1 Full surface wave equations

We consider the motion of a layer of fluid under the following simplifying assumptions:

- the fluid is *inviscid*, *incompressible* (density normalized to unity), and no surface tension;

- the bottom is flat, at depth $z = -H$;
- the fluid motion is *irrotational*, assumed to be uniform in the (horizontal) y -direction and unbounded in the x -direction; if the horizontal and vertical velocities are denoted by $U = U(x, z, t)$ and $W = W(x, z, t)$ respectively, irrotational motion means

$$U_z - W_x = 0$$

and allows the introduction of the fluid potential Φ such that

$$(U, W) = \nabla\Phi, \quad U = \Phi_x, \quad W = \Phi_z.$$

Then incompressibility implies

$$U_x + W_z = 0, \quad \Delta\Phi = 0;$$

- the surface elevation is the graph of a function (no overturning waves) $\eta = \eta(x, t)$.

Then the governing equations are

$$\Delta\Phi \equiv \Phi_{xx} + \Phi_{zz} = 0, \quad -H < z < \eta(x, t) \quad (6)$$

$$\Phi_z = 0 \quad \text{at } z = -H, \quad (7)$$

$$\partial_t\eta = -\eta_x\Phi_x + \Phi_z \quad \text{at } z = \eta(x, t), \quad (8)$$

$$\partial_t\Phi + \frac{1}{2}(\Phi_x^2 + \Phi_z^2) + g\eta = 0 \quad \text{at } z = \eta(x, t). \quad (9)$$

Equation (8) is a kinematic condition; equation (9) is a dynamic condition, resulting from Bernoulli's equation restricted to the free surface.

Remark 21 *Alternative descriptions*

1. For various reasons it is convenient to introduce the potential at the free surface

$$\varphi(x, t) = \Phi(x, \eta(x, t), t)$$

and its x -derivative (which is a velocity type of quantity)

$$u(x, t) = \partial_x\varphi = \Phi_x + \Phi_z\eta_x$$

Then $\partial_t\varphi = \Phi_t + \Phi_z\eta_t$, and the free surface conditions become

$$\partial_t\eta = -u\eta_x + w(1 + \eta_x^2), \quad (10)$$

$$\partial_t u = -\partial_x[g\eta + \frac{1}{2}u^2 - \frac{1}{2}w^2(1 + \eta_x^2)] \quad (11)$$

where w is the vertical velocity at the free surface:

$$w(x, t) = W(x, \eta(x, t), t).$$

This is a set of equations for η, u in which, however, w still has to be expressed as a function of η, u .

2. Another way to rewrite the kinematic surface condition (the continuity equation) is as a local conservation law:

$$\partial_t \eta = -\partial_x \int_{-H}^{\eta} \Phi_x dz \quad (12)$$

which shows that the flux equals the integrated horizontal velocity. Stated differently, this is nothing but mass-conservation.

3. This also shows that the boundary conditions are in 'conservation form': (12) and (11).
 4. Yet another interpretation of the kinematic surface condition is that the vertical fluid velocity should equal the vertical displacement of the fluid surface:

$$\Phi_z = \frac{d}{dt} \eta(x(t), t) \equiv \partial_t \eta + \partial_x \eta \frac{dx}{dt}$$

For *multi-directional waves*, depending on both horizontal variables, a simple extension is as follows.

Due to the irrotationality of the velocity field \vec{v} a scalar potential function Φ can be defined as $\nabla \Phi = \vec{v}$. Mass conservation within the fluid domain \mathcal{D} can now be expressed as Laplace's equation for the potential

$$\Delta \Phi \equiv \Phi_{xx} + \Phi_{yy} + \Phi_{zz} = 0 \quad \text{in } \mathcal{D}. \quad (13)$$

Now the two conditions that govern the free surface dynamics are

$$\Phi_t = -\frac{1}{2} |\nabla \Phi|^2 - g\eta \quad \text{on } z = \eta(x, t), \quad (14)$$

$$\eta_t = \Phi_z - \eta_x \Phi_x - \eta_y \Phi_y \quad \text{on } z = \eta(x, t). \quad (15)$$

Additional initial and boundary conditions are required to make the problem well-posed. For the applications in hydrodynamic laboratories, these are an impermeable bottom condition, lateral boundary conditions, absorption at the down stream end of the domain, and some prescribed condition at the upstream position to define a suitable signalling problem. Alternatively, on a spatially unbounded domain, an initial surface elevation and horizontal fluid velocity may be prescribed.

For a simple interpretation of the SWE's, most important is to observe how the interior Laplace problem is linked to the dynamic equations. The algorithm for one timestep can be described as follows:

- start with a given surface elevation and given potential at the surface;
- then solve the Laplace equation, and calculate the velocity ($\nabla \Phi$) at the free surface;
- use this information in the right hand side of the dynamic equations, and evolve these for one time-step;
- this then provides updated fluid surface and potential,

- start the next timestep.

The main problem in this algorithm is the calculation of the velocity at the free surface, actually the solution of the *Dirichlet to Neumann (DtN) problem*: given Φ at the surface, find $\nabla\Phi$ at the surface. Numerically this can be done nowadays quite efficiently and accurately. In finding simplified models for theoretical investigations, various different approximations for the solution of the DtN problem are used to arrive at equations on the free surface, thereby having eliminated the problem to calculate the interior flow. We will describe this in the next subsection.

3.1.1 Variational structure

Another way to interpret the dynamical structure is using a variational description. In fact, it has been observed (independently) by Zakharov (1968) and Broer (1974) and Miles (1977) that SWE can be described as a Hamiltonian system. Summarising, this can be described by using as variables the fluid potential at the free surface and the surface elevation. Then the full surface wave equations can be described as a Hamiltonian system (see for full details [4])

$$\partial_t\eta = -\delta_\phi H(\phi, \eta), \quad \partial_t\phi = \delta_\eta H \quad (16)$$

where H is the Hamiltonian functional and $\phi = \Phi|_{z=\eta}$ is the free surface potential. Just as for Hamiltonian systems from Classical Mechanics, the Hamiltonian is the sum of kinetic and potential energy

$$H(\phi, \eta) = K(\phi, \eta) + \int \frac{1}{2}g\eta^2 dx$$

where the kinetic energy is given for solutions of the Dirichlet problem for the Laplace problem in the fluid domain: $K(\phi, \eta) = \int \int \frac{1}{2}|\nabla\Phi|^2 dx dz = \int \phi [\partial_n\Phi]_{z=\eta} dx$. Since this functional cannot be expressed explicitly in terms of ϕ, η , which would require to solve the DtN problem, simplified models can be obtained by constructing approximations for this functional. In doing so, and taking as governing equations the system (16) with the approximated Hamiltonian, leads to a model that has retained the basic variational structure, which is not guaranteed in a direct approach.

3.2 Physics of wave evolution: energy, momentum

3.2.1 Intermezzo: Conservation laws and conserved quantities

We start with some general ideas about conservation in pde's, which will after that be applicable for the wave problems.

Let the state of a dynamic system be described by a function $u = u(x, t)$ of the spatial variable x and time t . Let $e = e[u]$ be some local density, i.e. an expression that depends on u in such a way that the value of e at (x, t) is determined by $u(x, t)$ and a finite number of x -derivatives of u at (x, t) . We write $e = e[u](x, t)$ for its value at (x, t) .

The integral of e along a given spatial interval $[a, b]$ defines the integrated quantity $E_{[a,b]}$ that will depend on u and time:

$$E_{[a,b]}[u](t) \equiv \int_a^b e[u](x, t) dx$$

In specific cases, depending on the evolution equation and the density, the time derivative may depend only on the value of a (local) flux density Q at the end points of the interval:

$$\frac{d}{dt}E_{[a,b]}[u](t) = -Q[u](b, t) + Q[u](a, t). \quad (17)$$

This is then called a *global conservation law* for the density e , and Q is called the *flux density* corresponding to e .

Rewriting the right hand side

$$-Q[u](b, t) + Q[u](a, t) \equiv - \int_a^b \partial_x Q[u](x, t) dx$$

and (assuming differentiability) the left hand side

$$\frac{d}{dt}E_{[a,b]}[u](t) \equiv \int_a^b \partial_t e[u](x, t) dx,$$

the global law can be rewritten like

$$\int_a^b \{ \partial_t e[u](x, t) + \partial_x Q[u](x, t) \} dx = 0.$$

If this holds for any interval of integration $[a, b]$ (within some given interval), it follows⁵ that

$$\partial_t e[u](x, t) + \partial_x Q[u](x, t) = 0. \quad (18)$$

This expression is called the *local conservation law* for the density e .

Remark 22 1. As described above, the local conservation law is derived from the global conservation law; the reverse is equally true (and simpler): integrating (18) along an interval $[a, b]$, the result will be (17).

2. When for a given solution, the net flux through the boundary vanishes, i.e. when

$$Q[u](a, t) = Q[u](b, t)$$

then

$$\partial_t \int_a^b e[u](x, t) dx = 0$$

and we have a conserved quantity or *constant of the motion*: $\int_a^b e[u](x, t) dx$.

3. In the special case that the evolution equation for the state variable itself is of the form of a local conservation law

$$\partial_t u(x, t) = -\partial_x Q[u](x, t)$$

it is custom to talk about an *evolution equation in conservation form*.

⁵Intuitively clear; strictly speaking use Lagrange's Lemma and assume continuity of the expression in brackets in the integral.

4. For a given evolution equation, and a local density e , the existence of a local/global conservation law is special; in general the density will satisfy a *local balance law* of the form:

$$\partial_t e[u] + \partial_x \Phi[u] = S[u]$$

where S is the so-called local *source density*.

For a system in *more spatial dimensions*, write $\mathbf{x} \in \Omega \subset R^n$ and let Ω be a bounded or unbounded domain with \mathbf{n} the outward pointing normal at the boundary $\partial\Omega$. The flux of a (scalar) density e is an n -vector \mathbf{Q} and the flux through the boundary is determined by the normal component:

$$\text{flux through boundary: } \int_{\partial\Omega} \mathbf{Q} \cdot \mathbf{n} dA$$

With a source density S , the global balance law reads

$$\frac{d}{dt} \int_{\Omega} e(\mathbf{x}, t) d\mathbf{x} = - \int_{\partial\Omega} \mathbf{Q} \cdot \mathbf{n} dA + \int_{\Omega} S(\mathbf{x}, t) d\mathbf{x}$$

Using Gauss' theorem:

$$\int_{\partial\Omega} \mathbf{Q} \cdot \mathbf{n} dA \equiv \int_{\Omega} \text{div } \mathbf{Q} d\mathbf{x},$$

and assuming smoothness, a local balance law is obtained in the form

$$\partial_t e + \text{div } \mathbf{Q} = S.$$

If $S = 0$, the balance law becomes a conservation law.

All these notions become particularly relevant when for $e(u)$ a physically motivated density is taken.

3.2.2 Conservation properties for full SW equations

1. *Conservation of mass (fluid)*: The 'continuity equation' in the description of continua with a mass density ρ and Eulerian velocity v reads

$$\partial_t \rho + \text{div}(\rho v) = 0,$$

expressing mass conservation: in a fixed domain Ω with boundary $\partial\Omega$ with normal n ; the total amount of mass can only change by flux through the boundary as is expressed as follows:

$$\partial_t \int_{\Omega} \rho dx = - \int_{\Omega} \text{div}(\rho v) dx = - \int_{\partial\Omega} \rho v \cdot n$$

For water, we assume $\rho = \text{constant}$, corresponding to

$$\text{div}(v) = 0,$$

which leads to Laplace equation with the expression for the Eulerian velocity (from irrotationality assumption) $v = \nabla \Phi$.

2. For the depth integration of mass-conservation the kinematic condition follows as we have seen already:

$$\partial_t \int_{-H}^{\eta} dz = \partial_t \eta = -\partial_x \int_{-H}^{\eta} \Phi_x dz$$

The flux density is the horizontal momentum, to be denoted by $I(x, t)$:

$$I = \int_{-H}^{\eta} \Phi_x dz$$

3. Total Energy

The local kinetic energy density is given by $\frac{1}{2}\rho|\nabla\Phi|^2$. The potential energy of mass ρ at height z equals ρgz , and therefore the total energy integrated over depth is found to be:

$$E(x, t) = \int_{-H}^{\eta} \left(\frac{1}{2}\rho|\nabla\Phi|^2 + \rho gz \right) dz = \int_{-H}^{\eta} \left(\frac{1}{2}\rho|\nabla\Phi|^2 \right) dz + \frac{1}{2}\rho g \eta^2 + \left(\frac{1}{2}\rho g H^2 \right)$$

We can and will neglect the inessential constant $\frac{1}{2}\rho g H^2$ in the following.

3.3 Linearised SW, dispersion

As stated above, any simplifying model is based on an approximation of the DtN problem. Without surface elevation and bottom variations, the problem is on a straight strip and can be solved in closed form by Fourier techniques. This explains the various approximations, which are based (given a horizontal straight bottom) on specifying simplifying properties of the surface elevation. In particular, for infinitesimally small amplitude waves, the linearised problem can be solved and leads to the basic (linear) dispersion relation between frequency and wavenumber, given by (using normalised variables)

$$\omega = \pm\Omega(k), \quad \text{with } \Omega(k) = k\sqrt{\tanh(k)/k}. \quad (19)$$

In more dimensions, for a plane wave with wavevector k , the same dispersion relation is found with $k = |k|$.

We now present the details of the derivation.

First we have to consider the linearised equations. This means, we suppose that the wave elevation η is small, and just as well the fluid velocity $\nabla\Phi$. Then consistently in lowest order, we retain only linear terms in the surface equations, and, moreover, take the boundary in the Laplace problem to be the undisturbed level $z = 0$. Then the full set becomes Laplace problem on strip:

$$\Delta\Phi \equiv \Phi_{xx} + \Phi_{yy} + \Phi_{zz} = 0, \quad -H < z < 0 \quad (20)$$

with boundary condition at bottom:

$$\Phi_z = 0 \quad \text{at } z = -H, \quad (21)$$

and linearised free surface conditions: kinematic surface condition

$$\partial_t \eta = \Phi_z \quad \text{at } z = 0, \quad (22)$$

and dynamic linearised surface condition

$$\partial_t \Phi + g\eta = 0 \quad z = 0. \quad (23)$$

To find the dispersion relation, we look for time harmonic solutions, periodic in the horizontal directions, i.e. both η and Φ of the form $e^{i(k_1 x + k_2 y - \omega t)}$. The general solution for Φ then has the form

$$\Phi(x, y, z, t) = a(z) e^{i(k_1 x + k_2 y - \omega t)}$$

and inserting in the equation there results:

$$a_{zz} - |k|^2 a = 0, \quad \text{with } |k| = \sqrt{k_1^2 + k_2^2}.$$

With the boundary condition at bottom (21), which requires $a(z, t) = 0$ at $z = -H$, the solution becomes:

$$a(z) = A \sinh(|k|(z + H))$$

with A arbitrary. Hence $\Phi = A \sinh(|k|(z + H)) e^{i(k_1 x + k_2 y - \omega t)}$.

For the kinematic surface condition (22) we need to calculate Φ_z at $z = 0$, which is $\Phi_z|_{z=0} = A|k| \cosh(|k|H) e^{i(k_1 x + k_2 y - \omega t)}$. Writing

$$\eta(x, y, t) = B e^{i(k_1 x + k_2 y - \omega t)}$$

the kinematic boundary condition requires:

$$-i\omega B = A|k| \cosh(|k|H) \quad (24)$$

while the dynamic boundary condition gives

$$-i\omega A \sinh(|k|H) + gB = 0. \quad (25)$$

These two conditions for the coefficients A, B only can give a nontrivial result provided

$$\omega^2 = g|k| \tanh(|k|H).$$

which is the desired dispersion relation.

In one space dimension, allowing the wave number to have different signs, the odd solution should be taken and there results the dispersion relation

$$\omega = |k| \sqrt{\frac{g \tanh(|k|H)}{|k|}}$$

Note the limiting behaviour, for small wave numbers (long waves) and large wave numbers (short waves)

$$\begin{aligned} \omega &\sim |k| \sqrt{gH} \quad \text{for } k \rightarrow 0, \\ \omega &\sim \sqrt{g|k|} \quad \text{for } k \rightarrow \infty. \end{aligned}$$

In more dimensions, given the wave vector, the positive value of ω is taken for waves travelling in the wave vector direction, and the negative sign for waves in the opposite direction.

3.4 KdV type of equations

One step further than the linear approximation, is to take for small amplitude solutions a first order nonlinear effect into account. At the same time, assumptions on the characteristic wave length are commonly made; mostly the restriction is to ‘long’ waves. A characteristic, often used approximation is the so-called Boussinesq approximation, which corresponds to the specific relation between the wave amplitude ε and wave length λ given by $1/\lambda^2 \sim \varepsilon$, the case of ‘rather small, rather long waves’. This is the basic assumption to arrive at what are called Boussinesq-type of equations. These equations describe both waves running to the right and the left. Further restricting to waves running mainly in one direction, then leads to KdV-type of equations⁶. The general form of these equations is a first order in time equation of the form

$$\partial_t u = -\partial_x (Ru + \frac{3}{4}u^2) \quad (26)$$

for the normalised surface elevation u . Here R is a linear operator that determines the specific dispersive properties, since the linearised equation has dispersion relation $\omega = kR(k)$. For the classical KdV equation, in the Boussinesq approximation, the operator is given by

$$R_{KdV}(k) = 1 + \frac{1}{6}\partial_x^2 \simeq 1 - \frac{1}{6}k^2$$

where the symbol \simeq means the action of the operator in Fourier space. With this choice, the dispersion is correct for long waves, since $\Omega(k) = k(1 - \frac{1}{6}k^2 + \dots)$ for $k \rightarrow 0$. Then the operator is a local operator, and KdV is a partial differential equation. An improvement of the dispersive properties can be achieved by taking for R the exact dispersion operator for linear waves, i.e.

$$R \simeq \sqrt{\tanh(k)/k}$$

Then the operator is no longer an ordinary differential operator and the equation (26) is no longer a standard partial differential equation. For modelling waves of shorter wave lengths, as in hydrodynamic laboratories, this improvement turns out to be essential. Observe, for instance, that for R_{KdV} the phase and group velocity become negative for shorter waves, very different from the exact relation for which both tend to zero for shorter waves. In finite difference approximations of (26) this non-local behaviour is a serious problem, and various improvements have been proposed and studied (for instance Pade-approximations). In the next subsection we will see explicitly the importance of the choice of the dispersion relation.

⁶*Korteweg-de Vries equation (1895)*

Korteweg and de Vries derived in 1895 a model equation for the motion of waves on the surface of a layer of fluid above a flat bottom. Restricting to rather low, rather long waves, they derived the equation (26) that now bears their name with $R_{KdV}(k)$. This equation became well known in the sixties since it turned out that from a mathematical point of view it was the first partial differential equation shown to be completely integrable, leading to a huge extension of the theory of nonlinear pde’s. It also became clear that many problems in physics and technics are modelled by this equation.

Being an evolution equation, first order in time, the *initial value problem* requires to find the evolution of the surface profile from a given initial profile. This initial value problem for KdV is not easy to solve; for arbitrary initial profiles, numerical calculations have to be used to find the subsequent wave profiles; the complete integrability makes it possible in principle to write down the time-asymptotic profile.

The quadratic nonlinearity in (26) is the second order term from the quadratic character of the original problem. However, the specific form is just a simplification and higher order terms could be added. This is actually done in an alternative model, the so-called Stokes expansion, in which a series expansion in the steepness of the wave, essentially ka , is taken as parameter. Then the equation has also a dispersive operator in the quadratic term. In view of the rather good performance of the model (26), almost up to the point of breaking waves, as will be shown in the next sections, we restrict to the non-dispersive quadratic nonlinearity for simplicity.

Finally, as stated above, a model should retain the Hamiltonian character of the full SWE's. Indeed, the KdV-type of equations have a Hamiltonian structure too, given by

$$\partial_t u = -\partial_x \delta_u H(u)$$

where the symplectic operator is the differential operator ∂_x and the Hamiltonian is now given by

$$H(u) = \int \left[\frac{1}{2} u R u + \frac{1}{4} u^3 \right] dx$$

In [4] a derivation of the KdV-equation is described using the variational structure as the guiding principle to obtain consistent simplified models.

3.4.1 Solitons of KdV

The motivation for Korteweg and de Vries to study the problem of surface waves, was to settle a dispute that continued throughout the nineteenth century about the existence of *travelling waves*: *is it possible that a wave exists that doesn't change in time, but is merely travells at a fixed speed?*

They showed, by deriving their (KdV-) equation and analyzing it, that the answer is affirmative. More so, it is possible to write down the wave shapes and speeds explicitly. This is quite unexpected at first sight, since KdV combines nonlinearity (leading to “breaking”-phenomenon) and dispersion (“spreading” of initial profile). The remarkable property is that these combined effects make it possible that there exist *travelling waves*, waves with a specific profile, say f , that will neither break nor spread (an exact balance between the counteraction of breaking and spreading), and that travel undisturbed in shape at a specific speed, say V . That is, a solution of the form

$$\eta(x, t) = f(x - V t)$$

just as in the translation equation, but now only for specific profiles f and specific velocity V .

To find the wave profile f and the velocity V , we substitute this form in the KdV-equation, in normalised variables

$$\partial_t \eta + \partial_x \left[\partial_x^2 \eta + \frac{1}{2} \eta^2 \right] = 0.$$

Then the pde becomes an ode for the function f in which V enters as a parameter to be determined together with the profile. We shall see that, in fact, there is a whole family of such waves; the higher the amplitude, the larger the velocity.

Writing $\xi := x - V t$, the equation becomes

$$-V \partial_{\xi} f(\xi) + f(\xi) \partial_{\xi} f(\xi) + \partial_{\xi}^3 f(\xi) = 0$$

A solution of this equation, for certain V , produces the wave profile f of the wave that travels undisturbed in shape at speed V .

3.4.2 Analysis of solitary wave profiles

To find the solution we have to distinguish two cases:

- *space-(and time-) periodic solutions*, for which f is a periodic function of ξ , the so-called cnoidal waves (since the profile is expressed with the elliptic cnoidal function), and
- *solitary wave solutions*: wave profiles of a single hump that decay, together with all derivatives, sufficiently fast at infinity (“almost confined”, exponentially small outside a certain interval).

We will concentrate on the solitary wave profiles.

Then by integrating the equation above once, noticing that the constant of integration has to vanish as a consequence of the decay at infinity, leads to the second order ode for the profile:

$$-V f(\xi) + \frac{1}{2} f(\xi)^2 + \partial_{\xi}^2 f(\xi) = 0$$

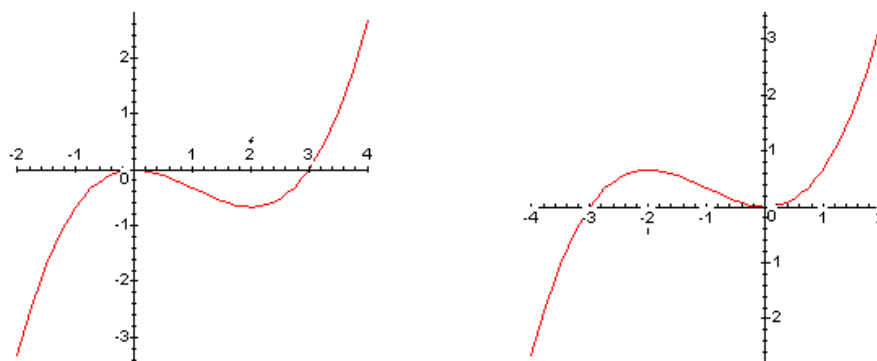
This equation can be solved in a standard way by observing the *mechanical analogue*: when ξ is interpreted as the time, and f as the position, the equation describes the motion of a particle of unit mass subject to a potential force with potential energy U according to Newtons law:

$$\partial_{\xi}^2 f(\xi) + \frac{dU}{df} = 0 \tag{27}$$

with potential energy

$$U(f) = -\frac{1}{2} V f^2 + \frac{1}{6} f^3.$$

The plot of U is qualitatively as shown below, at the left for positive values of V , at the right for negative values:



Looking for a solitary wave profile f that decays to zero for ξ tending to $-\infty, \infty$, we look for the solution that is nontrivial and connects the origin with itself: a *homoclinic orbit*. Clearly, this can only be achieved for positive values of V .

In more detail, for the profile equation *mechanical-energy conservation* holds. Multiplying (27) with $\partial_\xi f$ and integrating the equation again, there results:

$$\frac{1}{2} [\partial_\xi f]^2 + U(f(\xi)) = E.$$

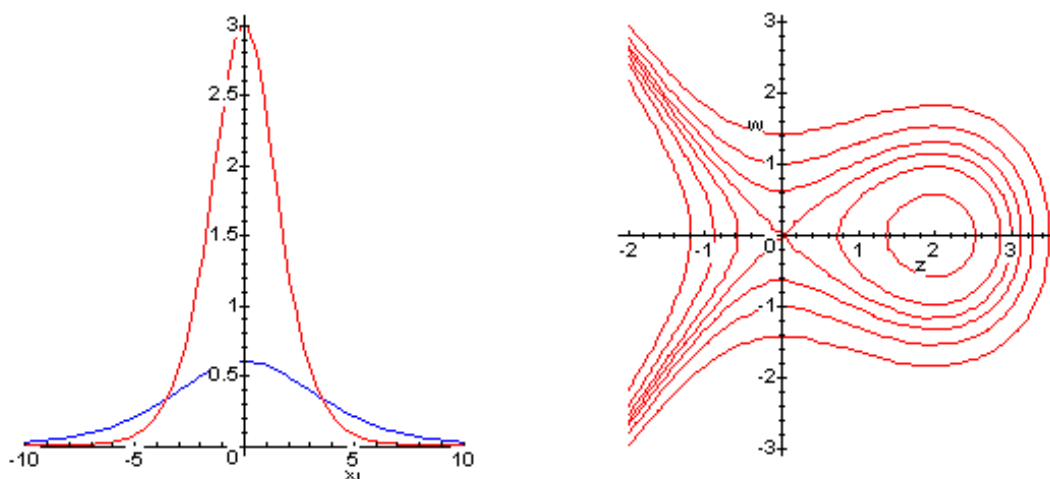
Since E should be zero for a solitary wave profile, the equation becomes

$$\frac{1}{2} [\partial_\xi f(\xi)]^2 - \frac{1}{2} V f(\xi)^2 + \frac{1}{6} f(\xi)^3 = 0.$$

This is a first order equation for the profile function and its solution can be given explicitly. This solution is a *solitary wave profile*: for each V , with $V > 0$, it is given by

$$f(\xi, V) = \frac{3V}{\cosh(\frac{1}{2} \sqrt{V} \xi)^2}$$

Two profiles, for $V = .2$ and $V = 1$, are shown below:



Observe: with V the velocity, the amplitude is proportional to V , and the width proportional to $\frac{1}{\sqrt{V}}$: the larger the amplitude, the more confined the wave, and the larger its speed.

The solution above can be found in the *phase plane* $z = f, w = \partial_\xi f(\xi)$ in the following way. The curves of constant energy, given by

$$\frac{1}{2} w^2 + U(z) = E$$

are sketched in the phase-plane (z, w) , and in this phase portrait the solitary wave corresponds to the homoclinic orbit which is the level curve through the origin (for which $E = 0$).

Exercise 23 The KdV-eqn in normalized form:

$$\partial_t u + u_{xxx} + uu_x = 0,$$

can be written as a conservation law:

$$\partial_t u = -\partial_x \left[u_{xx} + \frac{1}{2}u^2 \right],$$

and so u is a conserved density. In fact there are more conserved densities; three relevant conserved densities are given below. Verify the given corresponding fluxes:

$$\begin{aligned} e(u) &= u, & \text{mass} \\ f(u) &= u_{xx} + \frac{1}{2}u^2 \end{aligned}$$

$$\begin{aligned} e(u) &= u^2 & \text{momentum} \\ f(u) &= 2uu_{xx} - u_x^2 + \frac{2}{3}u^3 \end{aligned}$$

$$e(u) = \frac{1}{2}u_x^2 - \frac{1}{6}u^3, \quad \text{energy}$$

$$f(u) = -\frac{1}{2}u_{xx}^2 + u_x u_{xxx} + u_x^2 u - \frac{1}{2}u^2 u_{xx} - \frac{1}{8}u^4$$

For solutions decaying (with all derivatives) at infinity (or for periodic solutions), the global conserved quantities are the integrals over the whole real line (or with the integrals over one period, respectively). Determine these conserved quantities.

Exercise 24 Consider the so-called BBM eqn. (Benjamin, Bona & Mahony, 1972):

$$(1 - \partial_x^2)\partial_t u = -\partial_x u - u\partial_x u \tag{28}$$

This model equation is a variant of the KdV eqn (normalised variables).

1. Determine the dispersion relation of the linearised equation. What is the relation with the dispersion relation of the full SW eqn's, and with that of the standard-KdV-equation.
2. Looking for travelling waves, $u(x, t) = f(x - Vt)$, write down the equation for the profile function f ; do you recognise this (form of the) equation? Find the solution explicitly.

3.5 Focusing/defocusing NLS-models

In this subsection we derive the equation for the envelope of a wave group. In view of the applications of propagation in wave tanks, we will sketch the derivation of the spatial NLS-equation, in which the evolution parameter is in the down stream direction (instead of in time). Then the spatial evolution is expressed in terms of temporal derivatives; this is the convenient description for a signalling problem: sending waves from a specified point (the

wave maker) and investigating the down-stream evolution. This equation can be derived in a certain approximation as follows. Without the nonlinearity, the next equations are equivalent

$$\partial_t u + i\Omega(-i\partial_x)u = 0 \Leftrightarrow \partial_x u - iK(i\partial_t)u = 0$$

where the function K is the inverse of Ω , the wavenumber now taken to depend on the frequency:

$$k = K(\omega) \Leftrightarrow \omega = \Omega(k).$$

Now, with $i\Omega = \partial_x R$ as in (26), assume in lowest order that $R \approx 1$, so that approximately $\partial_t u + \partial_x u = 0$. Then, in this approximation we can replace $\partial_x(u^2)$ in (26) by $-\partial_t(u^2)$, leading to

$$\partial_x u - iK(i\partial_t)u - \partial_t(u^2) = 0, \quad (29)$$

where we removed the factor $\frac{3}{4}$ for convenience (by rescaling u).

Starting point is a given time signal at the initial position, centered at a central frequency $\bar{\omega}$. The result will be an NLS-equation with coefficients that are determined by the specific dispersion relation. The derivation given here follows the description in [6] (apart from some change of notation and corresponding changes in signs).

3.5.1 Linear dispersive envelope equation

First we deal with dispersive effects upon neglecting the quadratic nonlinearity. Then we include effects of the nonlinearity. We will do this in some detail, since the precise relation with the actual wave height u contains some intricate phase effects which are important. The general solution of the linearised equation can be written down as

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

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

$$u(x, t) = A(x, t) e^{i\Theta(\bar{\omega})} + cc,$$

where here and in the following we use the notation $\Theta(\omega)$ to denote the phase of a mode with frequency ω satisfying the dispersion relation

$$\Theta(\bar{\omega}) = K(\bar{\omega})x - \bar{\omega}t,$$

where K is the inverse of Ω : $K(\omega) = \Omega^{-1}(\omega)$. The complex amplitude that describes the modulation is given by

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

and satisfies the linear dispersive equation

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

To eliminate the first order term in the dispersion, a frame moving with the group velocity $1/K'(\bar{\omega})$ is introduced, i.e.

$$\tau = t - K'(\bar{\omega})x, \zeta = x.$$

Writing

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

the equation can then be rewritten like:

$$\partial_\zeta A - iK_2(i\partial_\tau)A = 0. \quad (30)$$

Exercise 25 *Linear envelope equation*

1. Show that K_2 is second order in ν :

$$K_2(\nu) = \beta\nu^2 + O(\nu^3);$$

determine β and show it is positive for surface wave dispersion. This coefficient is called the *group-velocity dispersion coefficient*; can you explain why?

2. Taking only the second-order approximation, the linear envelope equation (30) becomes

$$\partial_\zeta A + i\beta\partial_t^2 A = 0. \quad (31)$$

What is the relevance of the sign of β in this equation? This is a simple dispersive wave equation; what is the dispersion relation? Is there a conservation property (local conservation law, constant of the motion)?

3. Show that, in contrast to the so-called *diffusion equation* (when $\beta > 0$) for the real function u

$$\partial_\zeta u = \beta\partial_t^2 u$$

(a parabolic pde) is dissipative: Calculate for instance $\partial_\zeta \int (\partial_t u)^2 dt$ and show that it has damping solutions. So, very different from the equation (31) which is not dissipative but dispersive.

3.5.2 Nonlinear contributions

To incorporate nonlinearity in the deformation of the envelope amplitude, the generation of a second order double harmonic bound wave and a variation of the equilibrium level is anticipated:

$$u = A_0 e^{i\Theta(\bar{\omega})} + B e^{2i\Theta(\bar{\omega})} + C + cc. \quad (32)$$

The amplitudes A_0, B and C are allowed to vary slowly in the frame of reference, and B and C are of second order in the amplitude. It is natural to restrict to solutions u which are, either, square integrable in time (decaying at infinity) or are periodic with some period T . In the latter case $\int u dt = 0$, and the variations in the equilibrium level should satisfy at each position x

$$\int C dt = 0.$$

Inserting the Ansatz in the equation gives a residue that has to be made as small as possible. This defines the second order coefficients

$$B = 2\sigma_2 A_0^2, \text{ and } C = \sigma_0 [|A_0|^2 - I_0] \text{ with } I_0 = \int |A_0|^2 d\tau$$

where

$$\sigma_0 = \frac{1}{K'(\bar{\omega}) - K'(0)}, \sigma_2 = \frac{\bar{\omega}}{2K(\bar{\omega}) - K(2\bar{\omega})} \quad (33)$$

are (transfer) coefficients from the generation of the second harmonic and non-harmonic term in the solution. Then, to avoid resonant terms in third order, for A_0 there results the equation

$$\partial_\zeta A_0 + 4i\sigma_0 I_0 \bar{\omega} A_0 - iK_2(i\partial_\tau)A_0 + i\gamma |A_0|^2 A_0 = 0$$

with

$$\gamma = 4\bar{\omega} (\sigma_0 + \sigma_2). \quad (34)$$

One can simplify this result by getting rid of the term $4i\sigma_0 I_0 \bar{\omega} A_0$ in the equation by introducing an additional phase in A_0 :

$$A_0 = A e^{-4i\bar{\omega}\sigma_0 I_0 \zeta}$$

leading to the generalised NLS-equation, denoted by gNLS:

$$\partial_\zeta A - iK_2(i\partial_\tau)A + i\gamma |A|^2 A = 0. \quad (35)$$

The phase shift indicates that the physical solution should actually be seen in a frame of reference moving at a slightly adjusted speed; this effect is part of the nonlinear dispersion relation.

From a solution of this equation, the actual physical solution is then up to and including second order given by

$$u = A \exp i [\Theta(\bar{\omega}) - 4\bar{\omega}\sigma_0 I_0 \zeta] + \sigma_0 [|A|^2 - I_0] + 2\sigma_2 A^2 \exp i 2 [\Theta(\bar{\omega}) - 4\bar{\omega}\sigma_0 I_0 \zeta] + cc \quad (36)$$

This can be rewritten in a more attractive way by writing the complex amplitude A with real amplitude a and phase ϕ like $A = a e^{i\phi}$; then

$$u = 2a \cos(\Theta(\bar{\omega}) + \phi - 4\bar{\omega}\sigma_0 I_0 x) + 2\sigma_0 [a^2 - I_0] + 4a^2 \sigma_2 \cos(2(\Theta(\bar{\omega}) + \phi - 4\bar{\omega}\sigma_0 I_0 x)). \quad (37)$$

The non-harmonic term with σ_0 modifies locally the equilibrium level of the field (keeping the averaged value at zero), while the double harmonic term with σ_2 deforms the first-order harmonic profile to a cnoidal-type of profile.

In the envelope equation above, we have retained the full dispersive properties of the problem, just as in the KdV-type of equation in the previous subsection. 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 (26) 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 $\beta_2 = \frac{1}{2}K''(\bar{\omega})$, $\beta_3 = \frac{1}{6}K'''(\bar{\omega})$, and then A satisfies

$$\partial_\zeta A + i\beta_2 \partial_\tau^2 A - \beta_3 \partial_\tau^3 A + i\gamma |A|^2 A = 0. \quad (38)$$

Taking $\beta_3 = 0$ and performing a simple scaling transforms this equation to the standard form of the NLS-equation

$$\partial_\zeta A + i\partial_\tau^2 A + i\text{sign}(\beta_2\gamma)|A|^2 A = 0,$$

a well known equation that has been studied extensively (e.g. [1]). For this standard NLS, the quadratic function K_2 is even; with the third order dispersive term β_3 included, the equation is known as the Dysthe equation ([3]).

The sign of the coefficients, or better $\text{sign}(\beta_2\gamma)$, determines the character of the NLS equation:

- defocusing NLS if $\text{sign}(\beta_2\gamma) < 0$, and
- focusing NLS if $\text{sign}(\beta_2\gamma) > 0$.

The focussing NLS has soliton-type of solutions and more 'confined' solutions, as we shall see in the next section. In this case, the dispersive and the nonlinear effects counterbalance each other, while in the defocussing NLS the waves will spread.

For the problem under consideration it is important to realise that the sign depends on the value of the central frequency. In fact, for the surface wave dispersion, and also for the classical KdV long wave dispersion, the sign of β_2 is positive for each $\bar{\omega}$. However, as can be easily verified, for the full dispersion relation, the value of γ changes sign, being negative for $\bar{\omega} < \omega_{crit}$ and positive for $\bar{\omega} > \omega_{crit}$. The specific value of ω_{crit} is related to the critical wave number known as the Davey-Stewartson value, $k_{crit} \approx 1.363$. In contrast, when the long-wave dispersion as in the classical KdV equation is used, the value of γ is negative for all $\bar{\omega}$, leading to the defocusing NLS. This means that essentially different behaviour is found for these cases. This has as physical interpretation that when the wave length of the carrier wave is sufficiently large, the waves constituting a wave group have too little interaction to remain confined in a group, while for sufficiently short waves the interaction length covers several waves which leads to grouping behaviour.

Summary 26 For the spatial NLS as considered above, in laboratory coordinates the NLS equation reads

$$NLS - spat : (\partial_x + \frac{1}{V_0}\partial_t)A + i\beta\partial_t^2 A + i\gamma|A|^2 A = 0$$

In the same way we can derive the temporal NLS:

$$\begin{aligned} NLS - temp & : (\partial_t + V_0\partial_x)A + i\beta'\partial_x^2 A + i\gamma'|A|^2 A = 0 \\ \beta' & = V_0^3\beta; \gamma' = V_0\gamma \end{aligned}$$

3.5.3 Phase-amplitude equations for NLS

Writing

$$u(x, t) = 2a(x, t) * \cos(\Phi(x, t)) + \text{hot}$$

all of the above can also be written in terms of the

- real **amplitude** $a(x, t) = \sqrt{|A|^2}$, (defining the envelope) ; in many cases one uses the 'energy' $E = |A|^2$;

and

- quantities that define the carrier wave, namely the

phase	$\Phi(x, t) = k_0x - \omega_0t + \phi(x, t)$
local wave number	$k := \partial_x \Phi$
local frequency	$\omega := -\partial_t \Phi$

Notice that here we define the wavenumber and frequency as local quantities, to be determined from the phase.

Then NLS can be found from the following basic relations, the phase-amplitude relations:

<i>amplitude (energy)</i>	$\partial_t E + \partial_x(V(k)E) = 0$
<i>phase equation</i>	$\omega - \Omega(k) = \gamma E + \beta \frac{\partial_x^2 a}{a}$
<i>kinematic relation</i>	$\partial_t k + \partial_x \omega = 0$

where Ω is the standard linear dispersion relation, and

energy	$E = a^2$
groupvelocity	$V(k) = \Omega'(k)$
gr.vel. dispersion	$\beta = -\frac{1}{2}\Omega''(k) > 0$
transfer-coefficient	$\gamma > 0$

Remark 27 These equations have a variational structure. The Variational formulation is found from the Lagrangian functional

$$L = \int \int [(\omega - \Omega(k))a^2 + \beta a_x^2 - \frac{1}{2}\gamma a^4] dx dt.$$

Observe, in particular, the expression for the *Phase equation*, which has been written above like

$$\omega - \Omega(k) = \gamma E + \beta \frac{\partial_x^2 a}{a}$$

This is to be interpreted as an extension of '*nonlinear dispersion relation*' (NDR) which reads for one mode with amplitude q

$$\omega - \Omega(k) = \gamma q^2$$

The present modification results from the degeneracy caused by the ‘arbitrary’ choice of k_0, ω_0 , but, more important, NDR now includes an ‘envelope-profile’-dependence $\beta \frac{\partial_x^2 a}{a}$ from dispersion ($\beta \neq 0$), independent from magnitude but locally defined and dependent on the whole envelope.

Remark 28 The NDR can be written in an alternative form like

$$\beta \partial_x^2 a - \nu a + \gamma a^3 = 0, \text{ with } \nu = \omega - \Omega(k).$$

This form is particularly interesting when looking for steady state solutions, for which $\nu = \omega - \Omega(k)$ constant. As we shall see later, this equation has as simple mechanical analogy the dynamic (now ‘time’ is x) evolution of a particle with mass β in a potential force field as described by Newton’s equation. When ν is constant, the solutions are easy to find; when non-constant, the solutions may be very complicated, showing periodic, pseudo-periodic and even chaotic behaviour. This is at the heart of the complicated dynamics of surface waves!!

4 NLS-equation

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.

4.1 Math-physical structure

In the following we will consider for simplicity the sNLS, although most can easily be adapted to dNLS and gNLS.

The standard NLS-equation reads

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

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.

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).

4.1.1 Hamiltonian structure

The sNLS has a Hamiltonian structure of the following form:

$$\partial_\zeta A = i\delta H(A), \text{ with } H(A) = \int \left[\beta_2 |A_\tau|^2 - \frac{1}{2}\gamma |A|^4 \right] d\tau \quad (39)$$

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

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

4.1.2 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:

$$N(A) = \int |A|^2 d\tau,$$

with flow : $\partial_\zeta A = i\delta N(A) = iA$, i.e. $A = c.e^{i\zeta}$

The corresponding conservation law is of the form:

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

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

$$L(A) = \int i\bar{A}\partial_\tau A d\tau,$$

with flow : $\partial_\zeta A = i\delta L(A) = -\partial_\tau A$, i.e. $A(\zeta, \tau) = A(\zeta - \tau, 0)$

Corresponding conservation law:

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

4.2 Phase-Amplitude equations

4.2.1 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 29 *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).*

4.2.2 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 $\partial_t [f(t)e^{i\phi}] = [(\partial_t + i\phi_t) \circ f] \cdot e^{i\phi}$ 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

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

4.2.3 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

$$\partial_z E + \partial_t [K'(\omega_0 + \nu) \cdot E] = 0, \quad (40)$$

a variant of $\partial_t E + \partial_z(V E) = 0$, 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)

$$\text{NDR: } K(\omega) - k = \gamma E + \beta_2 \frac{a_{tt}}{a} \quad (41)$$

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

$$\partial_z \omega + \partial_t k = 0 \quad (42)$$

Remark 30 *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.*

4.2.4 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:

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

4.3 Coherent structures: special solutions

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.

4.3.1 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

$$K(\omega) - k \equiv \mu = \text{constant}. \quad (43)$$

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

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

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

$$\beta a_{\tau\tau} - \mu a + \gamma a^3 = 0 \quad (44)$$

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 :

$$\boxed{\beta \partial_\tau^2 a = -\frac{\partial}{\partial a} P(a), \text{ potential } P(a) = -\frac{1}{2}\mu a^2 + \frac{1}{4}\gamma a^4} \quad (45)$$

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 31 *The basic equation (45) can be scaled with a characteristic time T in τ and amplitude q :*

$$a'_{\tau'\tau'} - \mu' a' + p^2 a'^3 = 0, \quad \text{with } p = \sqrt{\frac{\gamma}{\beta}} q T;$$

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).

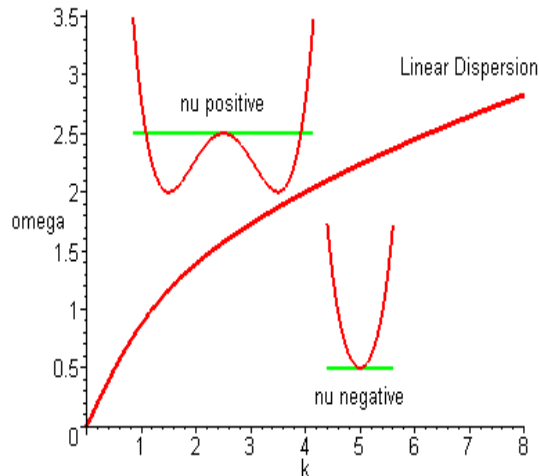
4.3.2 Dispersion plane, Steady soln's, evolution and instability

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,

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



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 $|a| < \sqrt{2}\sqrt{\frac{\mu}{\gamma}}$.

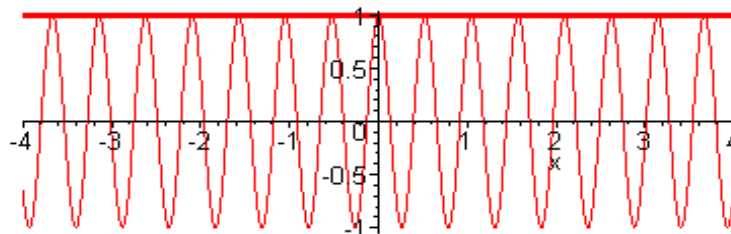
We now describe briefly the various solutions that can exist as is clear from the phase plane analysis.

4.4 Nonlinear harmonic

This is the solution with constant amplitude:

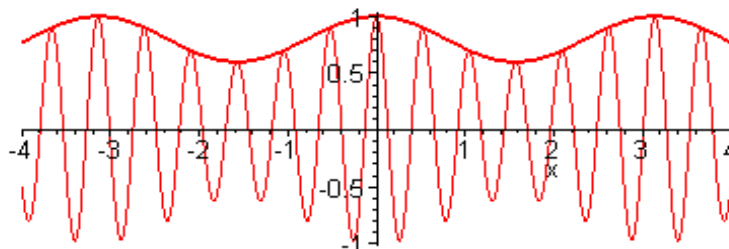
$$A = qe^{-i\gamma q^2 \zeta}$$

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:



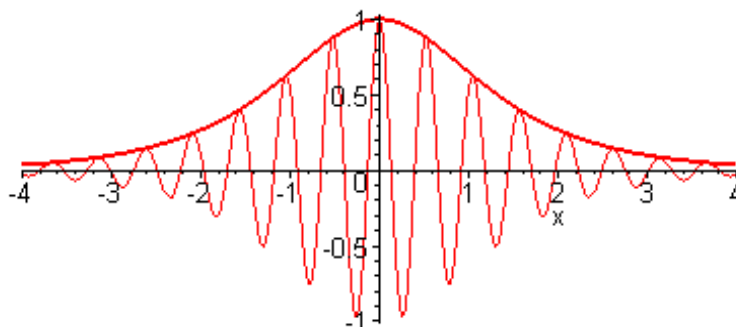
4.5 Nonlinear modulated harmonic

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:



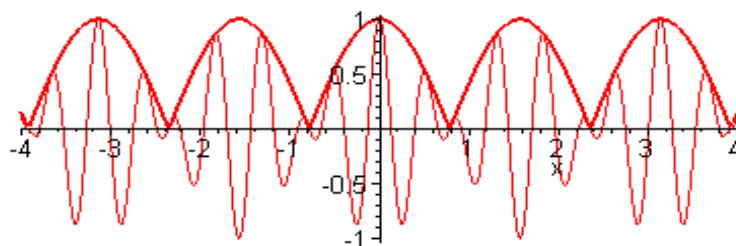
4.6 Soliton

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



4.7 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:



4.8 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

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

and then find for the dispersion relation:

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

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

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

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

Remark 32 *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 τ -periodic, ζ -soliton solution; the limiting behaviour of this soliton for $\zeta \rightarrow \pm\infty$ is the exponential growth and decay of the unstable linear expressions found here. See [1]!*

5 Numerical Methods: FD and FE

5.1 Finite difference method

5.1.1 Introduction

The basic idea underlying finite difference method is to replace the **differential** quotients in a differential equation by suitable **difference** quotients, (See [1]). In this introduction, we describe the following terms:

a. Difference schemes. A difference scheme is an approximation of a derivative at a point using the collective values of the nearby points. There are three main difference schemes:

- (i) **Centered scheme.** A centered scheme is a symmetric scheme about the point at which the derivative is being approximated. Example:

$$y'(x) \approx \frac{y(x+h) - y(x-h)}{2h}, \quad h \ll 1.$$

- (ii) **Forward difference scheme.** A forward difference scheme uses points 'ahead' of the point being approximated. Example:

$$y'(x) \approx \frac{y(x+h) - y(x)}{h}, \quad h \ll 1.$$

- (iii) **Backward difference scheme.** A backward difference scheme uses the points 'behind' the points being approximated. Example:

$$y'(x) \approx \frac{y(x) - y(x-h)}{h}, \quad h \ll 1.$$

b. Computational molecules. A computational molecule is a pictorial representation of a finite difference scheme for a partial differential equation in two independent variables.

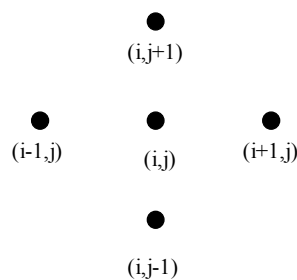


Figure 1: A computational molecule for $u_{xx} + u_{yy} = 0$

Figure (1) is a computational molecule for the approximation to the Laplace equation $u_{xx} + u_{yy} = 0$. Taking $\Delta x = \Delta y = h$ and a centered difference for both u_{xx} and u_{yy} , we obtain

$$u_{i,j} = \frac{1}{4}(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}) : .$$

A computational molecule for the finite approximation $u_t = u_{xx}$ in the form

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}$$

is shown in Figure (2).

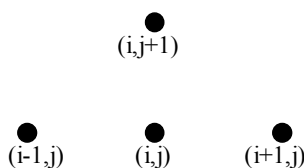


Figure 2: A computational molecule for $u_t = u_{xx}$

c. Grids. A grid is a set of points, called mesh points, in which the solution of a differential equation is approximated.

(i) A uniform grid: the points here are uniformly spaced

(ii) A non-uniform grid: the points are not uniformly spaced.

d. Explicit and Implicit methods. An explicit method is a method for which there is an explicit formula at a point for the value of the unknown terms appearing in the differential equation. An implicit method is one for which there is no explicit formula.

e. General multistep methods. Consider the first order differential equation $y' = f(x, y)$ defined on $[0, 1]$. The **general k-step method** for $y' = f(x, y)$ can be written as

$$N(y_n, y_{n+1}, \dots, y_{n+k}) = \sum_{j=0}^k \alpha_j y_{n+j} - h \sum_{j=0}^k \beta_j f(x_{n+j}, y_{n+j}) = 0, \quad (46)$$

where $\alpha_0 \neq 0$, y_n is an approximation to $y(x_n)$, $x_n = hn$, h is a small number called the step size.

In general the exact solution to the equation $y' = f(x, y)$ will not satisfy

$$N[y(x_n), y(x_{n+1}), \dots, y(x_{n+k})] = 0 : .$$

However for $h \ll 1$, α_i and β_j can be chosen such that

$$N[y(x_n), y(x_{n+1}), \dots, y(x_{n+k})] = h^{p+1} R_n + O(h^{p+2})$$

for some numbers p and R_n . If $p \geq 1$, then the method is said to be consistent, in this case p is called the order of the method.

Example. Consider the ordinary differential equation $y' = y^2$. Approximating y' using centered scheme, we have

$$y'(x_n) = \frac{y(x_{n+1}) - y(x_{n-1}))}{2h} + O(h^2).$$

Thus

$$\frac{y(x_{n+1}) - y(x_{n-1}))}{2h} - y^2(x_n) = O(h^2),$$

or

$$y(x_{n+1}) - y(x_{n-1}) - 2hy^2(x_n) = O(h^3).$$

The corresponding **explicit 2-step method** of order 2 is

$$N[y_{n-1}, y_n, y_{n+1}] = -y_{n-1} + y_{n+1} - 2hy_n^2 = 0$$

or

$$y_{n+1} = y_{n-1} + 2hy_n^2$$

Consistency of the finite difference scheme. A finite difference scheme is consistent if the truncation error tends to zero as the mesh is refined.

5.1.2 Finite difference method for ODE

We consider an ordinary differential equation in the form

$$u'(x) = f(x, u(x)) \quad ;, ;, x \leq x_0 \quad ;,$$

$$u(x_0) = u^0 \quad ; .$$

Let h be a uniform stepsize and $x_j = x_0 + jh \quad ;, ;, j = 1, 2, 3, \dots$. The following are examples of the numerical method for solving the above problem.

1. Euler Method

$$u_{n+1} = u_n + hf(x_n, u_n)$$

2. Midpoint Method $u_{n+1} = u_{n-1} + 2hf(x_n, u_n)$

3. Trapezoidal Method

$$u_{n+1} = u_n + \frac{1}{2}[f(x_n, u_n) + f(x_n, u_{n+1})]$$

The derivation of the methods can be obtained from difference ways such as finite difference scheme, geometrical consideration, Taylor series, numerical integration. The Euler method, as an example, can be obtained from the following approximation.

1. **Finite difference scheme.** The backward difference is used to approximate

$$y'(x)u'(x) \approx \frac{u_{n+1} - u_n}{h}$$

2. **Geometrical consideration.** The value of y_{n+1} is obtained via tangent line of the curve $u(x)$ at the point $x = x_n$. The equation of the tangent line is

$$y = f(x_n, u_n)(x - x_n) + u_n$$

and $u_{n+1} = y(x_{n+1})$.

3. **Taylor series.** The value $y(x_{n+1})$ is obtained by a truncation of a Taylor series near

$$x = x_n. u(x_{n+1}) = u(x_n) + hu'(x_n) + O(h^2)$$

4. **Numerical Integration.**

$$\int_{x_n}^{x_{n+1}} u'(x)dx = \int_{x_n}^{x_{n+1}} f(x, u(x))dx :,$$

and

$$\int_{x_n}^{x_{n+1}} f(x, u(x))dx \approx hf(x_n, u(x_n)) :,$$

to have

$$u(x_{n+1}) - u(x_n) \approx hf(x_n, u(x_n)) : .$$

In term of the general multistep method, the Euler is a one-step explicit method; the Midpoint is a two-step explicit method and the Trapezoidal is a one-step implicit method. The order of the method can be obtained by expanding $u(x_{n+1})$ into Taylor series near $x = x_n$ and this gives 1, 2, 1 for Euler, Midpoint, and Trapezoidal respectively.

5.1.3 Stability analysis by examples

We consider the simplest model hyperbolic partial differential equation

$$u_t + bu_x = 0 \quad , \quad b, s \text{ constant } :> 0,$$

$$u(0, x) = f(x),$$

$$u(t, 0) = g(t).$$

There are various finite difference forms for $u_t + bu_x$, (See [2]).

Let us consider the central-central difference, often called **leap-frog** formula, of the form

$$\frac{u_{r+1,s} - u_{r-1,s}}{2h} + b \frac{u_{r,s+1} - u_{r,s-1}}{2k} = 0 : . \quad (47)$$

Let $\rho = \frac{bh}{k}$, which is known as the Courant number. The equation (47) can be written as

$$u_{r+1,s} = u_{r-1,s} - \rho :: (u_{r,s+1} - u_{r,s-1}) : . \quad (48)$$

This method is an **explicit method** in variable t .

Carrying out a von Neumann stability analysis, let $u_{r,s} = \xi^r e^{i\beta ks}$, and substituting into (48) we obtain

$$\xi = \xi^{-1} - \rho(e^{i\beta k} - e^{-i\beta k}).$$

Using the Euler identity $e^{i\beta k} - e^{-i\beta k} = 2i \sin \beta k$, we have

$$\xi = \xi^{-1} - 2\rho i \sin \beta k,$$

or

$$\xi^2 + (2\rho i \sin \beta k)\xi - 1 = 0.$$

The roots of this equation (which are the amplification factors) are

$$\xi = -i\rho \sin \beta k \pm \sqrt{1 - \rho^2 \sin^2 \beta k}.$$

The method is stable if $|\xi| \leq 1$, that is the initial numerical error is not amplified in each step of the calculation. The stability of this leap-frog formula requires $|\rho \sin \beta k| \leq 1$. Assuming that $\sin \beta k$ may achieve its max/min value then

$$\rho \leq 1 \quad \text{or} \quad h \leq \frac{k}{b} : .$$

is the **stability condition** for the formula.

The truncation error for this leapfrog formula, can be obtained through Taylor series expansion. Let

$$\begin{aligned} u_{r+1,s} &= [u + hu_t + 1/2h^2u_{tt} + O(h^3)]_{r,s} \\ u_{r-1,s} &= [u - hu_t + 1/2h^2u_{tt} + O(h^3)]_{r,s} \\ u_{r,s+1} &= [u + hu_x + 1/2k^2u_{xx} + O(k^3)]_{r,s} \\ u_{r,s-1} &= [u - hu_x + 1/2k^2u_{xx} + O(k^3)]_{r,s} \end{aligned}$$

Substituting into (48), we obtain

$$2hu_t + 2\rho ku_x = O(h^3, k^2h) :,$$

or

$$u_t + bu_x = O(h^2, k^2).$$

Thus the **truncation error** is $O(h^2, k^2)$, we write as $O(2, 2)$.

Let us come back to the finite difference

$$u_{r+1,s} = u_{r-1,s} - \rho(u_{r,s+1} - u_{r,s-1}). \quad (49)$$

So far we have seen that the method is conditionally stable and has a good accuracy, $O(2,2)$. To initiate the use of this algorithm both $u_{0,s}$ and $u_{1,s}$, ($s = 0, 1, 2, \dots, N, N + 1$) has to be available. But neither $u_{1,s}$ ($s = 1, 2, \dots, N$) nor $u_{r,N+1}$, for any r , are specified. For $u_{1,s}$, we may use

$$u_{1,s} = u_{0,s} - \frac{bh}{2k}(u_{0,s+1} - u_{0,s-1}) + O(h^2, k^2) \quad , \quad s = 1, 2, \dots, N,$$

while for $u_{r,N+1}$, we may choose one of the following approaches.

$$u_{r,N+1} = u_{r,N}$$

or

$$u_{r,N+1} = \frac{1}{2}(u_{r+1,N} + u_{r-1,N}).$$

The first approach leads to

$$u_{r+1,N} = u_{r-1,N} - \rho(u_{r,N} - u_{r,N-1}), \quad (50)$$

while the second approach leads to

$$u_{r+1,N} = \frac{\rho/2 - 1}{\rho/2 + 1}u_{r-1,N} - \frac{\rho}{\rho/2 + 1}u_{r,N-1} \quad (51)$$

A von Neumann stability analysis on each equation yields

$$\xi - \frac{1}{\xi} + \rho[(1 - \cos \beta k) + i \sin \beta k] = 0,$$

and

$$\xi + \frac{\rho/2 - 1}{\rho/2 + 1} \frac{1}{\xi} - \frac{\rho}{\rho/2 + 1} e^{-i\beta k} = 0,$$

respectively. It is not difficult to see that (50) is **unstable** and (51) is **conditionally stable**. This is to illustrate that care must be used in selecting finite difference approximations.

5.1.4 Some examples

Example 1 : Linear Model for Run-Up Waves A linear model for one dimensional run up waves (monochromatic) may be written in the following form

$$\begin{aligned} \frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x}(hU) &= 0 \\ \frac{\partial U}{\partial t} + f^{(b)}\omega U &= -g \frac{\partial \eta}{\partial x} \end{aligned} \quad (52)$$

Here η and U are wave elevation and horizontal velocity, respectively. The uneven bottom is denoted by h . $f^{(b)}$ is the parameter related to the bottom friction, g is the gravity and ω is the wave frequency [See Figure 3].

A finite difference code for the problem can be written as

$$\begin{aligned} \frac{\eta_{i,k+1} - \eta_{i,k-1}}{2\Delta t} &= -U_{i,k} \frac{h_{i+1} - h_{i-1}}{2\Delta x} - h_i \frac{U_{i+1,k} - U_{i-1,k}}{2\Delta x} \\ \frac{U_{i,k+1} - U_{i,k-1}}{2\Delta t} &= -f_{i,k}^{(b)}\omega U_{i,k} - g \frac{\eta_{i+1,k} - \eta_{i-1,k}}{2\Delta x} \end{aligned}$$

A finite difference approximations for the right hand sides of the phase amplitude equations may be written as

$$2\beta\left[\left(\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}\right)\left(\frac{E_{i+1} - E_{i-1}}{2\Delta x}\right) - E_i \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta x)^2}\right] \quad (56)$$

$$\beta\left(\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}\right)^2 - \gamma E_i - \beta\left(\frac{a_{i+1} - 2a_i + a_{i-1}}{(\Delta x)^2}\right)/(a_i) \quad (57)$$

Care must be taken when computing the last term in the above finite difference scheme (57)

Example 3 : A Boussinesq model for surface gravity waves In this subsection we

consider a bi-directional model for surface gravity waves called a Boussinesq model. First let us consider gravity waves on a layer of fluid over a flat bottom. We assume that the fluid is ideal: inviscid, incompressible, density normalized to unity. Futhre it is assumed that the fluid motion is irrotational. This implies that velocity of fluid particles can be written as the gradient of a velocity potential. Here we consider to space dimension: one vertical and one horizontal, which coordinate z and x respectively. Let (x, z) be the spatial coordinate and t denote time. Let $\Phi(x, z, t)$ be the velocity potential and $\varphi(x, t) = \Phi(x, \eta(x, t), t)$. Let $\eta(x, t)$ and $u(x, t) = \varphi_x$ be the time dependent free surface and horizontal velocity, respectively [See Figure 4].

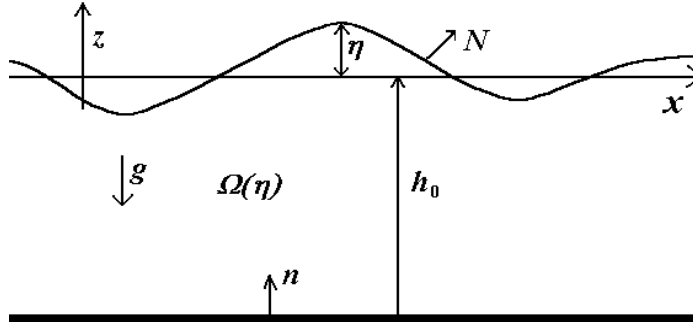


Figure 4: The fluid domain for a layer of water above a flat bottom at $z = h_0$ with free surface described as a function $z = \eta(x, t)$.

Assuming that the fluid is ideal, $\Phi(x, z, t)$, satisfies Laplace equation:

$$\Delta\Phi = 0 \quad \text{in } \Omega(\eta) \quad (58)$$

On the bottom, the normal component of the velocity is zero:

$$\nabla\Phi \circ n = 0$$

while on the free surface the kinematic and dynamic boundary conditions are

$$\eta_t = -u\eta_x + (1 + \eta_x^2)w \quad (59)$$

$$u_t = -\frac{\partial}{\partial x}[g\eta + \frac{1}{2}u^2 - \frac{1}{2}(1 + \eta_x^2)w^2] \quad (60)$$

The equations describing the boundary conditions on the free surface above are not in a closed form, they contain an expression $w = \Phi_z(x, z, t)$, $z = \eta(x, t)$ that has to be evaluated by solving the Laplace equation defined over the interior water domain. A Boussinesq model that we consider here, is a bi-directional model describing the quantities on the surface only. In principle, the vertical derivatives of the velocity potential w has to be approximated. There are many ways to derive this model, one of them leads to the following equations

$$\frac{\partial \eta}{\partial t} = -\frac{\partial}{\partial x}(u\eta) - \frac{\partial}{\partial x}(Ru) \quad (61)$$

$$\frac{\partial u}{\partial t} = -g\frac{\partial \eta}{\partial x} - u\frac{\partial u}{\partial x} \quad (62)$$

Here w is approximated by $-\frac{\partial}{\partial x}(Ru) - \eta u_x$. The operator R is an integral operator related to Fourier symbol $\hat{R} = \frac{\tanh kh_0}{k}$,

$$Ru(x, t) = \int_{-\infty}^{\infty} r(x-y)u(y, t)dy \quad , \quad r(z) = -\ln\left[\frac{\tanh(\frac{\pi z}{4h_0})}{\pi}\right]$$

A finite difference code for the right hand side of (61),(62), can be formulated as

$$\begin{aligned} -u_i \frac{\eta_{i+1} - \eta_{i-1}}{2\Delta x} - \eta_i \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{(Ru)_{i+1} - (Ru)_{i-1}}{2\Delta x} \\ -g \frac{\eta_{i+1} - \eta_{i-1}}{2\Delta x} - u_i \frac{u_{i+1} - u_{i-1}}{2\Delta x} \end{aligned}$$

5.1.5 Exercises

Excercise # 1

The Euler and Mid-point methods for solving an ODE

$$u'(x) = f(x, u) \quad , \quad u(0) = u^0$$

can be written as

$$u_{n+1} = u_n + hf(x_n, u_n),$$

$$u_{n+1} = u_{n-1} + 2hf(x_n, u_n),$$

respectively. Here we take $u_0 = u^0$. For the Mid-point method to initiate the procedure the values u_0 and u_1 should be available. This value u_1 can be first obtained using the Euler method.

1. Consider the ODE $u'(x) = -u$, $u(0) = 1$

- (a) Design a numeric code (pascal) to calculate u using the Euler method.
- (b) Same question in (a) but using the Mid-point method.
- (c) Compute u using (a) and (b) by taking different step-sizes h for each procedure and $0 \leq x \leq 3$.
- (d) Compare the result of (a), (b) and the exact solution.
- (e) Comment on the error of the computation and do some analysis.

Excercise # 2

We consider a kineal model of run up waves

$$\begin{aligned}\frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x}(hU) &= 0 \\ \frac{\partial U}{\partial t} + f^{(b)}\omega U &= -g\frac{\partial \eta}{\partial x}\end{aligned}$$

- (a) Start with a flat bottom and a constant parameter f^b , design numerical code for the model (including some boundary as well as initial conditions) on the spatial domain $[0, L]$, and $t \geq 0$.
- (b) Design a non flat bottom and modify the code in (a)
- (c) Improve the code in (b) by adding a point source at $x = 0$ (may be considered as a wave generator).

5.2 The finite element method

5.2.1 What is the finite element method?

The finite element method is a numerical technique to obtain an approximate solution to a wide variety of engineering problems. In a continuum problem of any dimension, the field variable (temperature, displacement, stress, etc.) posses infinitely many values as it is a function of each generic points in the solution region. Consequently, the problem has infinitely number of unknowns. The finite element procedure discretizes the problem by dividing the solution region into a finite number of elements and expressing the unknown field variable in term of approximating functions called **interpolation functions**. This approximating functions are defined in terms of the values of the field variable at specific points called **nodes**. The nodal values of the field variable and the interpolation functions for the elements completely define the behaviour of the field variable within the elements. In the finite element procedure the nodal values of the field variable becomes the new unknowns. Once these values are found, the field variables are expressed using the interpolation functions throughout the essemblege elements.

As we have studied the **finite difference method**, this method envisions the **solution region as an array of grid points**. The **finite element method**, on the otherhand, envisions the **solution region as built up of many small, interconnected elements**. Thus unlike the finite difference model which gives a point-wise approximation to the governing equations, the finite element model give a piecewise approximation to the equations. The

basic premise of the finite element method is that a solution region can be analytically modeled or approximated by replacing it with an assemblage of discrete elements, (See [4]).

Even though the finite element technique can solve quite difficult problems, a disadvantage of this method is that it becomes hard to use when it encounters an irregular geometry or unusual specification of boundary conditions. The finite element method, however, can be used to represent an exceedingly complex shape as the discrete elements modeled for a solution region can be put together in many different ways.

The finite difference and finite element method can be used to represent a complex geometrical shape of a device. For this device we may want to calculate a distribution of the temperature for a given thermal loading. Using a uniform finite difference mesh, the device would be reasonably covered but the boundary condition has to be approximated by a series of horizontal and vertical lines. The finite element model for this example would need a fewer nodes for a better approximation to the region. Further, it gives a better approximation to boundary values as the curve boundary shape is approximated by a series of straight lines. There are four different approaches to formulate the properties of each individual element.

1. Direct Approach
2. Variational Approach
3. Weighted Residual Approach
4. Energy Balance Approach

Regardless the approach we choose, the solution of a continuum problem by the finite element method always follows the step-by-step below.

1. Discretization of the continuum
2. Selection of the interpolation functions
3. Evaluation of the matrices of the elements by finding the element properties using one of the four approaches mentioned above
4. Assembling the matrices of the elements to obtain the system equations
5. Application of the boundary conditions
6. Solving the system equations
7. Making additional computations

In this study we will mostly use the variational approach. Using this approach, the third, fourth, and sixth step may be elaborated as follows.

- 3.a.** Writing the differential equations as a variational principle.

- 3.b.** Approximating the unknown field variable in the variational principle by linear combination of the functions defined for the finite elements, say $u(\mathbf{x}) \approx u_N(\mathbf{x}) = \sum_{k=1}^{k=N} c_k \phi_k(\mathbf{x})$. In this case c_k are unknowns and have to be determined.
- 3.c** Constructing the element matrices, element by element.
- 4.** Assembling the matrices of the elements together into a global stiffness matrix \mathbf{A} and a load vector \mathbf{f} to find the quadratic functional of the form $I[u_N] = \mathbf{c}^T \mathbf{A} \mathbf{c} - 2\mathbf{c}^T \mathbf{f}$.
- 6.** Relating the minimization of the variational principal to the minimization of the quadratic functional $I[u_N] = \mathbf{c}^T \mathbf{A} \mathbf{c} - 2\mathbf{c}^T \mathbf{f}$. When \mathbf{A} is symmetric then the minimization of this quadratic functional will occur when \mathbf{c} is the solution to the system $\mathbf{A} \mathbf{c} = \mathbf{f}$. In general the matrix \mathbf{A} will be a sparse matrix.

In this section we will consider two examples on the application of the finite element method on boundary value problems. The first example is for a second order ODE and the second is for a Laplace equation. In both examples we use the **variational approach** in slightly different manners: in the first example we minimize the resulting global matrix expression $I(N)$, while in the second example we use $\delta I = 0$ to find the element matrix equation, here I is variational expression for the problem.

5.2.2 Finite element method by examples

Example 1: A finite element approximation for a linear ODE Consider the following second order linear ordinary differential equation:

$$L[u] = -\frac{d}{dx}\left(p(x)\frac{du}{dx}\right) + q(x)u = f(x) \quad (63)$$

defined on the interval $0 \leq x \leq 1$ and satisfying the natural boundary conditions

$$u(0) = u_0 \quad , \quad u(1) = u_1 \quad (64)$$

To simplify the problem, we assume that p and q are constant.

Finding the finite approximation to the solution, we first make a discretization of the domain, (See [1]). For simplicity, we set up a uniform grid of $N + 2$ points on the interval $0 \leq x \leq 1$, say $x_k = kh$, where $h = \frac{1}{N+1}$ and $k = 0, 1, 2, \dots, N+1$. Define the k^{th} element to be (x_k, x_{k+1}) . Since each of the element has two nodes, we choose the interpolation function to be linear. Hence on the finite element k , i.e. for $x_k \leq x \leq x_{k+1}$, the interpolation function is

$$\varphi_k(x) = a_k x + b_k.$$

Let c_k and c_{k+1} be the value of $\varphi_k(x)$ at $x = x_k$ and $x = x_{k+1}$, respectively. Then

$$\varphi_k(x) = \frac{x_{k+1} - x}{h} c_k + \frac{x - x_k}{h} c_{k+1}. \quad (65)$$

Now, consider the function $\phi_k(x)$ defined on $[0, 1]$.

$$\phi_k(x) = \begin{cases} \frac{x-x_{k-1}}{h} & : x_{k-1} \leq x \leq x_k \\ \frac{x_{k+1}-x}{h} & x_k \leq x \leq x_{k+1} \\ 0 & \text{otherwise} \end{cases}$$

$k = 1, 2, 3, \dots, N$ [See Figure ()].

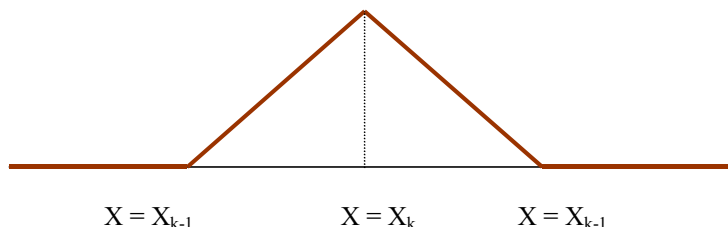


Figure 5: The hat function

From (65) and (??), on the finite element k (i.e. for $x_k < x < x_{k+1}$) the solution $u(x)$ can be approximated by $\varphi_k(x)$,

$$\begin{aligned} u(x) \approx \varphi_k(x) &= \phi_k(x)c_k + \phi_{k+1}(x)c_{k+1} \\ &= [\phi_k(x) \ :: \ \phi_{k+1}(x)] \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} \end{aligned} \quad (66)$$

Using the Variational Approach, let

$$I[u] = \int_0^1 [p(u'(x))^2 + qu^2(x) - 2f(x)u(x)]dx \quad (67)$$

then

$$\delta I = 2 \int_0^1 [pu'(x)\delta u' + (qu(x) - f(x))\delta u]dx : . \quad (68)$$

Using an integration by parts, we obtain

$$\delta I = -2 \int_0^1 [pu'' + qu - f(x)]\delta u dx + 2[pu_x \delta u]_{x=0}^{x=1}.$$

The function u that minimizes the functional $I[u]$, must satisfy $\delta I = 0$. Because δu is an arbitrary admissible variation, assuming that $u_x(0) = u_x(1) = 0$, the necessary conditions for $u(x)$ to minimize $I[u]$ yield

$$-pu''(x) + qu(x) = f(x)$$

We approximate this minimizing function $u(x)$ by a linear combination of $\phi_k(x)$.

$$u(x) \approx u_N(x) = \sum_{k=1}^N \phi_k(x)c_k, \quad (69)$$

where the unknown $\{c_k\}_{k=1}^{k=n}$ must be determined. Once the $\{c_k\}$ are known the approximation of $u(x)$ at any point can be obtained from (69).

From (68), on the finite element k, $pu'(x)\delta u' + (qu(x) - f(x))\delta u$ can be approximated by

$$p\varphi'_k(x)\delta\varphi'_k(x) + [q\varphi_k(x) - f(x)]\delta\varphi_k(x), \quad (70)$$

where

$$\begin{aligned} \varphi_k(x) &= [\phi_k(x) \ \phi_{k+1}(x)] \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} \\ \varphi'_k(x) &= \left[\frac{-1}{h} \ \frac{1}{h} \right] \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} \\ \delta\varphi_k(x) &= [\phi_k(x) \ \phi_{k+1}(x)]\delta \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} \\ \delta\varphi'_k(x) &= \left[\frac{-1}{h} \ \frac{1}{h} \right]\delta \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} \end{aligned}$$

Further, on the finite element k, we approximate $f(x)$ by $f(x) = \phi_k(x)f_k + \phi_{k+1}(x)f_{k+1}$. Thus on the finite element k, from (68), we obtain

$$\begin{aligned} \int_{x_k}^{x_{k+1}} pu'(x)\delta u' + (qu(x) - f(x))\delta u dx &\approx \int_{x_k}^{x_{k+1}} p\varphi'_k(x)\delta\varphi'_k(x) + [q\varphi_k(x) - f(x)]\delta\varphi_k(x) dx \\ &= I_k^s + I_k^m - I_k^l, \end{aligned} \quad (71)$$

where

$$\begin{aligned} I_k^s &= \int_{x_k}^{x_{k+1}} p\varphi'_k(x)\delta\varphi'_k(x) dx = \delta[c_k \ c_{k+1}]K_k^s \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} \\ I_k^m &= \int_{x_k}^{x_{k+1}} q\varphi_k(x)\delta\varphi_k(x) dx = \delta[c_k \ c_{k+1}]K_k^m \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} \\ I_k^l &= \int_{x_k}^{x_{k+1}} f(x)\delta\varphi_k(x) dx = \delta[c_k \ c_{k+1}]F_k, \end{aligned}$$

Thus on the finite element k, $x_k < x < x_{k+1}$

$$\begin{aligned} &\int_{x_k}^{x_{k+1}} pu'(x)\delta u' + (qu(x) - f(x))\delta u dx \\ &\approx \delta[c_k \ c_{k+1}]K_k^s \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} + \delta[c_k \ c_{k+1}]K_k^m \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} - \delta[c_k \ c_{k+1}]F_k \end{aligned} \quad (72)$$

$$\approx \delta[c_k \ c_{k+1}] \left\{ S_k \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} - F_k \right\} \quad (73)$$

S_k is the local stiffness matrix for the k^{th} element .

From (67) and (69)

$$\begin{aligned}
\delta I[u] \approx \delta I[u_N] &= \int_0^1 pu'(x)\delta u' + (qu(x) - f(x))\delta u dx \\
&= \sum_{k=0}^N \int_{x_k}^{x_{k+1}} p\varphi'_k(x)\delta\varphi'_k(x) + [q\varphi_k(x) - f(x)]\delta\varphi_k(x) dx \\
&= \sum_{k=0}^N \delta[c_k :: c_{k+1}] \left\{ S_k \begin{bmatrix} c_k \\ c_{k+1} \end{bmatrix} - F_k \right\} \approx 0
\end{aligned}$$

giving

$$\mathbf{S}\mathbf{c} = \mathbf{F}.$$

for a global stiffness matrix \mathbf{S} , vectors \mathbf{c} and \mathbf{F} . Thus the problem is reduced into finding the solution of a system of linear equations.

Example 2. A finite element approximation for a Laplace equation The following example is adapted from [5]. Here, we consider the following 2-D Laplace equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0, \quad \Omega \quad (74)$$

with boundary conditions

$$u = u^0, \text{ on } S_1; \quad \frac{\partial u}{\partial n} = 0, \text{ on } S_2, \quad (75)$$

where $S_1 \cup S_2$ is the total boundary of Ω .

First let us discretize the problem by dividing Ω into triangular elements, and then find the **element matrices**. On a single element, say the k^{th} element, we can propose an interpolation function

$$\varphi_k = \alpha_1 + \alpha_2 x + \alpha_3 y; \quad (76)$$

which varies linearly in x and y and produces three unknowns per element. These unknowns can be related to nodal values at nodes 1, 2, and 3 [See Figure (6)]. Let c_1^k, c_2^k, c_3^k be the values of u at the nodes 1, 2, 3 respectively.

Then

$$\begin{bmatrix} c_1^k \\ c_2^k \\ c_3^k \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix}, \quad (77)$$

or

$$\mathbf{c}^k = \mathbf{M}^k \boldsymbol{\alpha}; \quad (78)$$

The inverse of (77) gives the relationship between $\boldsymbol{\alpha}$ and \mathbf{c}^k ,

$$\begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \frac{1}{2A} \begin{bmatrix} 2A_1^0 & 2A_2^0 & 2A_3^0 \\ b_1 & b_2 & b_3 \\ a_1 & a_2 & a_3 \end{bmatrix} \begin{bmatrix} c_1^k \\ c_2^k \\ c_3^k \end{bmatrix};$$

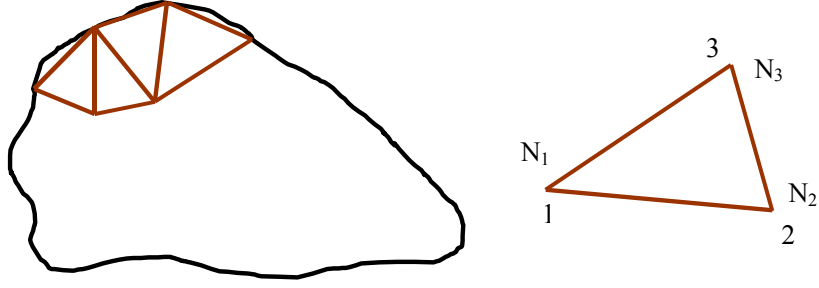


Figure 6: A finite element discretization, local numbering, and global numbering

or

$$\boldsymbol{\alpha} = (\mathbf{M}^k)^{-1} \mathbf{c}^k ;,$$

where

$$\begin{aligned} a_i &= x_k - x_j ; \quad b_i = y_j - y_k ; \quad 2A_i^0 = x_j y_k - x_k y_j ; \\ i &= 1, 2, 3 \quad , \quad j = 2, 3, 1 ; \quad k = 3, 1, 2; \\ 2A &= b_1 a_2 - b_2 a_1, \end{aligned}$$

here A is the area of the element.

From (76) and (??), φ_k and $\delta\varphi_k$ can be written as

$$\varphi_k = \phi_1 c_1^k + \phi_2 c_2^k + \phi_3 c_3^k = \Phi^T \mathbf{c}^k, \quad (79)$$

$$\delta\varphi_k = \Phi^T \delta\mathbf{c}^k ;, \quad (80)$$

where $\phi_i = \frac{1}{2A}(2A_i^0 + b_i x + a_i y)$; $i = 1, 2, 3$ and $\Phi = (\phi_1 \quad \phi_2 \quad \phi_3)^T$. We may compute the derivatives of φ_k to obtain

$$\begin{aligned} \frac{\partial\varphi_k}{\partial x} &= \alpha_2 = \frac{1}{2A}(b_1 c_1 + b_2 c_2 + b_3 c_3) = \frac{1}{2A} \mathbf{b}^T \mathbf{c}^k, \\ \frac{\partial\varphi_k}{\partial y} &= \alpha_3 = \frac{1}{2A}(a_1 c_1 + a_2 c_2 + a_3 c_3) = \frac{1}{2A} \mathbf{a}^T \mathbf{c}^k, \end{aligned} \quad (81)$$

where $\mathbf{a} = (a_1 \quad a_2 \quad a_3)^T$, $\mathbf{b} = (b_1 \quad b_2, \quad b_3)^T$ and $\mathbf{c}^k = (c_1 \quad c_2 \quad c_3)^T$. Similarly

$$\begin{aligned} \frac{\partial\delta\varphi_k}{\partial x} &= \frac{1}{2A} \mathbf{b}^T \delta\mathbf{c}^k \\ \frac{\partial\delta\varphi_k}{\partial y} &= \frac{1}{2A} \mathbf{a}^T \delta\mathbf{c}^k. \end{aligned} \quad (82)$$

Using Variational Approach, let

$$I = \frac{1}{2} \int \int [(\frac{\partial u}{\partial x})^2 + (\frac{\partial u}{\partial y})^2] dx dy - \int_{S_2} q u dS. \quad (83)$$

The minimizing function u for this $I(u)$ satisfies ($\delta I = 0$)

$$\int \int \left[\frac{\partial u}{\partial x} \frac{\partial \delta u}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial \delta u}{\partial y} \right] dx dy = 0 \quad (84)$$

On the k^{th} element, $u \approx \varphi_k$, $\frac{\partial u}{\partial x} \approx \frac{\partial \varphi}{\partial x}$, $\frac{\partial u}{\partial y} \approx \frac{\partial \varphi}{\partial y}$ and $\delta u \approx \delta \varphi_k$. Substituting (79), (80), (81) and (82) into (84) we obtain

$$\frac{1}{4A^2} \int \int [\mathbf{b}\mathbf{b}^T + \mathbf{a}\mathbf{a}^T] dx dy \mathbf{c}^k = 0 \quad (85)$$

After integration the left hand side of the above expression becomes

$$\mathbf{K}^k \mathbf{c}^k,$$

where $\mathbf{K}^k = \frac{1}{4A^2} [\mathbf{I} + \mathbf{J}]$,

$$\mathbf{I} = \begin{bmatrix} b_1^2 & b_1 b_2 & b_1 b_3 \\ b_1 b_2 & b_2^2 & b_2 b_3 \\ b_1 b_3 & b_2 b_3 & b_3^2 \end{bmatrix},$$

$$\mathbf{J} = \begin{bmatrix} a_1^2 & a_1 a_2 & a_1 a_3 \\ a_1 a_2 & a_2^2 & a_2 a_3 \\ a_1 a_3 & a_2 a_3 & a_3^2 \end{bmatrix}.$$

which is the local stiffness matrix for the k^{th} element. Contribution of this local stiffness matrix to the global stiffness matrix can in principle be seen from the local and global numbering. Let 1,2,3 be the local numbering of the nodes in the k^{th} element and let these number correspond to the global numbers N_1, N_2, N_3 . Let Stf be the global stiffness matrix, then

$$Stf[N_i, N_j] \Leftarrow K^k[i, j] \quad , \dots \text{ for } i, j = 1, 2, 3$$

We note that \mathbf{Stf} is a symmetric matrix. The boundary condition $u = u^0$ may be applied on the global system while keeping the symmetric property of the matrix \mathbf{Stf} .

5.3 Exercises

Excercise # 3

1. Consider a positive definite system of equations of the form

$$\mathbf{A}\mathbf{x} = \mathbf{f}$$

Let a_{ij} terms be the coefficients of the positive definite matrix \mathbf{A} , f_i terms be the coefficients of the vector \mathbf{f} , x_i be the coefficients of the unknown vector \mathbf{x} . In inditional notation, we may write

$$a_{ij}x_j = f_i \quad ; \quad i, j = 1, 2, \dots, n.$$

(a) Write an algorithm to solve this system of equations using Gaussian elimination.

- (b) Write a code in pascal for the algorithm in (a).
- (c) Try this solver for different matrices \mathbf{A} and vectors \mathbf{f} (e.g. \mathbf{A} is an upper triangular matrix, a lower triangular matrix, etc.). Start with $n = 2$ and gradually increase n .
2. Let \mathbf{A} be symmetric and banded $n \times n$ matrix and m be the band width. Noting that \mathbf{A} is symmetric, one needs only to store the diagonal and upper diagonal elements (within the band) of the matrix \mathbf{A} . Modify the solver for the system of equations $\mathbf{A} \mathbf{x} = \mathbf{f}$ in Question 1 to work only with the coefficients of the matrix \mathbf{A} within the band (the coefficients of \mathbf{A} outside the band are zero).
3. Apply the solver in (2.) to a global system obtained from finite element approximation to

$$\frac{d^2 u}{dx^2} = x - x^2$$

defined on the interval $0 \leq x \leq 1$ and satisfying the natural boundary conditions

$$u(0) = u(1) = 1$$

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