Stability and Mobility of Localized and Extended Excitations in Nonlinear Schrödinger Models

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Alltjämt frågande skall jag vara framme där livet klingar ut – en klar enkel ton i tystnaden.

– Dag Hammarskjöld
Abstract

This thesis is mainly concerned with the properties of some discrete nonlinear Schrödinger equations. These naturally arise in many different physical contexts as the limiting form of general dynamical lattice equations that incorporate non-linearity and coupling. Interest is focused on theoretical models of coupled optical waveguides constructed from materials with a nonlinear index of refraction. In arrays of waveguides the overlap of the evanescent electric field of the modes in neighbouring waveguides provides a coupling and the nonlinearity of the material provides a mechanism to halt the discrete diffraction that otherwise would spread localized energy across the array. In particular, waveguide structures where also a nonlinear coupling is taken into account are studied. It is noted that the equation for the evolution of the complex amplitudes of the electric field along an array of waveguides also can be used to describe the dynamics of Bose-Einstein condensates trapped in a periodic optical potential. Possible excitations in arrays in both one and two dimensions are considered, with emphasis on the effects of the nonlinear coupling.

Localized excitations are considered from the viewpoint of the theory of discrete breathers, or intrinsic localized modes, i.e., solutions of the dynamical equations that are periodic in time and have a spatial localization. The general theory of such solutions, that appear under very general circumstances in nonlinear lattice equations, is reviewed. In an array of waveguides this means that light can propagate along the array confined essentially to one or a few waveguides. In general a distinction is made between excitations that are centred on a waveguide, or site in the lattice, and excitations that are centred inbetween waveguides. Usually only the former give stable propagation. When the localized beam can be displaced to neighbouring waveguides the array can operate as an optical switch. With the inclusion of nonlinear coupling between the sites, as in the model derived in this thesis, the stability of the site-centred and bond-centred solutions can be exchanged. It is shown how this leads to the existence of highly localized mobile solutions that can propagate transversely in the one-dimensional array of
waveguides. The inversion of stability of stationary solutions occurs also in the two-dimensional array, but in this setting it fails to give good mobility of localized excitations. The reason for this is also explained.

In a two-dimensional lattice a discrete breather can have the form of a vortex. This means that the phase of the complex amplitude will vary on a contour around the excitation, such that the phase is increased by $2\pi S$, where $S$ is the topological charge, on the completion of one turn. Some ring-like vortex excitations are considered and in particular a stable vortex with $S = 2$ is found. It is also noted that the effect of charge flipping, i.e., when the topological charge periodically changes between $-S$ and $S$, is connected to the existence of quasiperiodic solutions.

The nonlinear coupling of the waveguide model will also give rise to some more exotic and novel properties of localized solutions, e.g., discrete breathers with a nontrivial phase. When the linear coupling and the nonlinear coupling have opposite signs, there can be a decoupling in the lattice that allows for compact solutions. These localized excitations will have no decaying tail. Of interest is also the flexibility in controlling the transport of power across the array when it is excited with a nonlinear plane wave. It is shown how a change of the amplitude of a plane wave can affect the magnitude and direction of power flow in the array.

Also the continuum limit of the one-dimensional discrete waveguide model is considered with an equation incorporating both nonlocal and nonlinear dispersion. In general continuum equations the balance between nonlinearity and dispersion can lead to the formation of localized travelling waves, or solitons. With nonlinear dispersion it is seen that these solitons can be nonanalytic and have discontinuous spatial derivatives. The emergence of short-wavelength instabilities due to the simultaneous presence of nonlocal and nonlinear dispersion is also explained.
Populärvetenskaplig sammanfattning


Det är mot denna bakgrund som det teoretiska arbetet i denna avhandling har utförts. Mer specifikt har en matematisk modell av diskreta icke-linjära Schrödingerekvationer för kopplade vågledare, ordnade både i en och två dimensioner, studerats. Speciellt tungt har lagts vid effekten av icke-linjära kopplningar mellan vågledarna och det är snarare egenskaperna hos olika lösningar till dessa ekvationer som varit av intresse än de möjliga faktiska tillämpningarna. Syftet med avhandlingen är därför också att få bättre förståelse för de allmänna egenskaperna
hos i första hand diskreta icke-linjära dynamiska ekvationer. Utgångspunkten har varit teorin för intrinsiskt lokaliserte moder (eng. "discrete breathers"), d.v.s. lösningar till ekvationerna som är periodiska i tiden och lokaliserte i rummet, och som existerar under mycket allmänna villkor i icke-linjära system. De viktigaste forskningsresultaten inkluderar observationen att i modellen för vågledare med icke-linjär koppling kan skifte i stabilitet mellan lösningar som är lokaliserte på en vågledare och lösningar som är lokaliserte mellan vågledare leda till lösningar som lätt kan röra sig tvärs över raden av vågledare. Detta gäller i en dimension, medan det i två dimensioner visar sig mycket svårt att ästadkomma rörliga lösningar. Vi visar också hur den icke-linjära kopplingen kan leda till att ljus strikt kan lokalisera till en eller flera vågledare utan koppling till de intilliggande. Även andra mer komplicerade excitationer i både en och två dimensioner studeras, där fasen på det elektromagnetiska fältet i respektive vågledare är av stor betydelse. Vidare visas hur man genom att samtidigt skicka ljus i alla vågledare (en plan våg) enkelt kan styra i vilken riktning energi transportereras mellan vågledarna.
When you work with a project, long and hard over days, weeks, months and years, you never quite realize that at some point you will be finished. There are days of joy and inspiration; days of setbacks and despair; days when you are a genius (or think you are); days that become night – and day again; days when you feel utterly privileged to work with something you really enjoy; but never is there a day when you can imagine the feeling of being finished. In a way you never will, but you might be lucky enough to some day feel content. Yet, this thesis marks the end of something, being it perhaps only to a strive for a degree. It is certainly not complete, nor could it possibly ever become given more time, but I believe it has reached a point where it will just have to do as it is.

**Thesis outline**

The study of arrays of waveguides constructed from materials with nonlinear optical properties, which is the background for most of the theoretical work in this thesis, is mainly motivated from their possible use as switches in all-optical communication networks and computers, where light is manipulated by light itself. Nonlinear effects are integral for the operation of such devices. An important step on the way towards all-optical communication is the use of propagating nonlinear localized waves (solitons) for high bit-rate information transfer in optical fibres, that has led to a major increase in the transmission speed of large quantities of data. Currently, much research is also devoted to the processing and steering of light beams, with future prospects for optical integrated circuitry. In this context the study of discrete systems is interesting since optical waves will experience a periodic refractive index and therefore have many similarities with electrons in semiconductor crystals.\(^1\) The first theoretical work on nonlinear waveguide arrays was done two decades ago and the experimental verification of spatially localized waves 

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\(^1\)See further examples in the review article [46] and the book [114].
optical pulses came ten years later. Different techniques have been suggested on how to steer an optical pulse between different waveguides, and part of our work is aimed in this direction by considering how the inclusion of nonlinear coupling between the waveguides affects the properties of excitations. The main efforts of our research, however, have been directed towards understanding the fundamental properties of nonlinear coupling and nonlinear dispersion, rather than devoted to applications. This has spurred our rather unrestricted investigations into existence, stability and mobility of nonlinear modes, and, maybe a bit surprisingly from the approach taken, the subsequent discovery of some effects that may have important applications.

The aim of this presentation is two-fold. Firstly, it gives an account of the research I have participated in over the past years, culminating in the included papers in Part I. Secondly, it serves to give an introduction to this research, and to the nonlinear localization aspect of the field of nonlinear science. As such the introductory Part I of the thesis gives the background necessary to understand the papers. It is written bearing in mind the knowledge of an advanced undergraduate student in physics having no prior experience of the subject. Reading it will hopefully bring an appreciation and understanding of the generality of the concept of nonlinear localization, as well as an orientation on some commonly used methods.

Part I – Introduction

The first chapter gives a brief introduction to the origin of nonlinear models and discusses how energy localization in the form of solitons and discrete breathers can be possible in such models. This chapter contains the basic theory of nonlinear localization and should be pretty much self-contained. It gives a broader overview of the theory than needed for the papers, and serves to give a general introduction to the topic. In Chapter 2 the model equation that is the main focus of the papers is derived, both in the context of coupled optical waveguides and for a Bose-Einstein condensate in a periodic potential. Chapter 3 then discusses the mathematical properties of the equations, and of their solutions, with focus on symmetries and conservation laws. Finally, Chapter 4 contains some comments on the papers and an outlook for further investigations.

Part II – Publications

This part consists of a collection of research papers that I have co-authored. These are introduced below, together with a short description of my own contributions to each paper.

Paper I: Enhanced mobility of strongly localized modes in waveguide arrays by inversion of stability

Background and contribution: The model for an array of waveguides with nonlinear coupling was originally derived in the Master Thesis of AE in 1995, supervised by MJ, where also its ability to support discrete solitons was investigated. Starting in 2001 this model was reinvestigated within the theory of discrete breathers in my own Master Thesis, also supervised by MJ. The discovery of stability inversion during this work hinted at mobility, and further investigation confirmed this. For the paper, I developed the code, performed all numerical simulations and wrote the text, except the major part of the conclusions.

Paper II: Nonlocal and nonlinear dispersion in a nonlinear Schrödinger-type equation: exotic solitons and short-wavelength instabilities


Background and contribution: This work was initiated during a one-year visit to the Technical University of Denmark in Lyngby and the group of PLC in 2003. Based on previous research, YuG suggested that the investigation of both nonlocal and nonlinear dispersion could be interesting since these effects earlier only had been studied separately. I did the analytical calculations, after an idea by YuG to use an auxiliary Hamiltonian, and performed all simulations for the continuum equation. Much effort was directed towards resolving the rather odd short-wavelength instabilities of solitons observed in the numerics. These could be understood by an analysis of the modulational instability of plane waves. The derivation in Appendix B was made by MJ, who also performed the simulations for the discrete system in Sec. 5. I wrote the manuscript, except Appendix B.

Paper III: Phase twisted modes and current reversals in a lattice model of waveguide arrays with nonlinear coupling


Background and contribution: Noting that the compact solutions discovered in paper II also could have a non-trivial phase, I thought it was interesting to investigate the further implications of this new property of localized modes. After I connected this property to the form of the norm current density for the discrete equation with nonlinear coupling, it was straightforward work to obtain other complex solutions. I made all calculations and wrote a draft for the manuscript that was condensed by MJ before submission.
Paper [IV] Stable stationary and quasiperiodic vortex breathers with topological charge $S = 2$


**Background and contribution:** The first results for this paper were obtained while testing the code developed for paper [V] by comparing with results of the well-known cubic DNLS equation. A bit surprisingly, I found a stable vortex with topological charge $S = 2$, and this spurred further investigation. The calculations for the quasiperiodic solutions (Fig. 4) were done by MJ and all other calculations were done by me, who also wrote the manuscript.

Paper [V] Stability, mobility and power currents in two-dimensional waveguide arrays with nonlinear coupling


**Background and contribution:** With the many interesting properties discovered in papers [I] and [III] for the one-dimensional array it was a natural extension to consider the same issues in higher spatial dimensions. In the spring of 2005 I was on a visit to Edinburgh hosted by Chris Eilbeck. During this visit, which included access to the Edinburgh Parallel Computing Centre, most of the calculations for this paper were performed.

Related publications of interest, but not included in the thesis.


**Acknowledgements**

Hopefully someone will find the work in this thesis useful and pick up where I left off or veer off in some other fruitful direction. Should any errors be revealed, they are solely on my account and not on any of the host of people who have made this
thesis possible. They all deserve my gratitude and, at the risk of leaving someone out, I would like to especially mention a few names.

First, and foremost, I would like to thank my supervisor Docent Magnus Johansson, always smiling, always inspirational, and always in the mood for discussion. I am glad he introduced me to the field of nonlinear science a few years ago, and for ever since having patiently shared his vast knowledge on the subject. There is no doubt that he is the perfect supervisor, especially after when he in times of limited funding selflessly left Linköping for new adventures abroad, simply to ensure my future existence as a doctoral student. For this I am ever in his debt. I am also grateful for the scrutinizing reading of this manuscript that has generated many constructive remarks and suggestions for improvements.

To Professor Peter Christiansen and Professor Yuri Gaididei I owe many thanks for taking such good care of me during my stay at the Graduate School of Nonlinear Science at the Technical University of Denmark in Lyngby during 2003. It was truly a privilege to learn some tricks-of-the-trade from these experts. I am also very grateful to Professor Chris Eilbeck for useful discussions and pleasant hiking experiences in the hills around Edinburgh during my visit to the Mathematics Department at Heriot-Watt University in 2005. Financial support from the EC Marie Curie Fellowship Programme and the HPC-EUROPA project is greatly acknowledged in connection with these visits, as well as general funding from the Swedish Research Council (Vetenskapsrådet).

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Michael Öster
Linköping, January 2007
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Part I

Introduction
CHAPTER

Nonlinear localization

Over the last few decades a shift of paradigm has taken place in the modelling of many phenomena, towards appreciating more complex relations between cause and effect. This shift can be thought of as turning from a reductionist perspective of the whole as the sum of its parts to a holistic view where the whole is greater (or lesser) than the sum of its parts. The former rests on the convenient but often unrealistic assumption that complicated causes can be resolved into more simple components, the effects of which are treated separately. This generally leads to linear models, the analysis of which is greatly simplified by the principle of superposition. However, the observation of phenomena that fall outside the predictions of linear models has led to the modelling of processes where cause and effect are not as easily distinguished. Although being one of the most fundamental conceptual changes in science over the past century this has gone by largely unnoticed as a revolution in thinking, mainly because it has been a slow process over many years involving many researchers from very diverse fields of science. Thus in areas such as physics, biology, chemistry, economy, medicine, mathematics and even psychology, there has been, and still is, a growing appreciation of nonlinear models and the qualitatively new phenomena emerging as a result of the study of these models. The highly interdisciplinary field of nonlinear science thus involves, among others, the study of deterministic chaos, the apparently random behaviour of well-defined systems perhaps most widely known through the 'butterfly effect'; fractals, objects that are self-similar on arbitrarily small length-scales; pattern formation, which, e.g., addresses the universality of many patterns in nature, such as the branching of trees, meandering rivers, the

\[1\] A very nice introduction to the field of nonlinear science is given in the book by A. Scott [182] and the impact of nonlinear modelling is evident from the volume [159], edited by the same author.

\[2\] See also the entry 'Butterfly effect' in [183] for some historical remarks.
spots on a leopard and the growth of form in a biological embryo, and how these can be mimicked by qualitative models; and systems biology, that takes a holistic approach to biology and medicine and describes cells and organisms as interactive networks of processes.

Of special interest are the formation, persistence and dynamics of structures that are spatially or temporally coherent, and whose emergence are the result of some entangled relation between cause and effect. An early lucid account of such a process was given by L.D. Landau in 1933 when he described the trapping of electrons in a crystal lattice \[128\]. As the electron moves through the lattice it experiences a periodic potential from the ions of the lattice due to Coulomb interaction, but the mutual interaction will also cause the presence of the electron to distort the lattice, i.e., to change the surrounding potential. If this distortion is sufficiently large a potential well is created and the electron can become trapped in the lattice. This bound state of electron and lattice distortion is known as a polaron, and its formation has no distinct cause \[3\] but is rather the result of the balance of interaction between electron and lattice. A physical model, that will capture the prominent features of this phenomenon, is to describe the motion of the electron wave packet by the Schrödinger equation with a potential that depends on the positions of the ions in the lattice. Then we also write down equations for the dynamics of the positions of the ions, may they be classical or quantum mechanical depending on our chosen level of detail, that will also depend on the position of the electron. In any form, the potential for the electron wave function will, through the dependence on the lattice coordinates, effectively depend on itself. Thus arises a nonlinear model to describe the polaron. In this context we may speak of the electron as being self-localized.

The formation of a polaron exemplifies how nonlinearity enters into our models as a way to deal with causality loops. Another example is the Einstein equations of general relativity, a set of ten coupled nonlinear partial differential equations that describes the curvature of space-time. The necessity with which nonlinearity enters into the equations can be well understood by the words of J.A. Wheeler: "Matter tells space how to curve and space tells matter how to move" \[149\]. Again, cause and effect cannot be clearly separated. We should note that there is no way to a priori prescribe a process in nature as being linear or nonlinear. It is not even a valid statement to make, since an attribute of linearity or nonlinearity can only be assigned to the model we derive to describe the process. Consider, e.g., the interference of light, where we can linearly superpose the amplitudes of the electric fields to get the resultant field but where no such easy treatment is possible if our model instead uses the intensity as the relevant quantity. Although this example may seem trivial, it actually touches upon an important relation between linear and nonlinear models. The intensity holds less information about the light than does the amplitude, since there is no knowledge of the phase of the electric field and this is integral to the correct understanding of interference. Thus the nonlinearity in the intensity is a consequence of a reduction of variables. We may then ask the question: Is it always possible to come up with a linear model? I

\[3\] Does the polaron form because there is an electron present to distort the lattice or is it because the lattice distortion is present to trap the electron?
will not presume to try and answer this question, but there is a relevant point that
starting even in a linear theory we may end up with nonlinear models on a lower
level of detail. As an example consider the interaction of light with matter. In a
quantum field model the electric field and the atoms are represented by a set of
quantized states that can be occupied by photons and electrons, respectively. The
relevant physical properties of the system can then be derived from the distribution
of these particles over the states, and interactions taken into account by transitions
between the states. This problem will be linear in the state of the electric field,
i.e., in the occupation of photons in each state, and the introduction of a new
field (a new source of light) will simply mean adding the occupation numbers for
each state. In a classical description we are not concerned with the individual
photons, but instead with the amplitude of the electric field at different frequencies
of oscillation, a quantity that is proportional to the square root of the average
occupation number of the photon states. The interaction of this field with the
atoms results in a change of the amplitude, corresponding to the annihilation
and creation of photons in different states. However, on the quantum level of
description some processes simultaneously involve two or more photons and the
occupation of intermediate, or virtual, states. From the classical viewpoint the
information of the individual photons is not available, and a two-photon process
will look as if the field has interacted with itself. Thus when the number of variables
is reduced, as we go from a quantum field description to a classical description,
the self-interaction implies a nonlinear model for the electric field. In this case
there is also a correspondence between the degree of nonlinearity and the number
of photons in the transitions. Two-photon processes give terms quadratic in the
electric field, three-photon processes give cubic terms, etc.

These examples serve to illustrate how nonlinearity enters into our physical
models, mainly as the result of the self-interaction of some entity. The correlation
of numerous predictions and observations also shows that nonlinearities are
a proper way to model these phenomena. For the dynamics of structures that are
coherent over time or space, nonlinear models have led to accurate descriptions
of many naturally occurring phenomena such as the propagation of large water
waves, energy transport in biomolecules, electric signals in nerve fibres, Jupiter’s
great Red Spot and the dynamics of domain walls in ferromagnetic materials.
This ubiquity of nonlinear waves underlines the importance of understanding the
mechanisms from which they appear, and only more so by the subsequent advances
in technology following from this understanding, e.g., the utilization of localized
light pulses (solitons) in fibre optic communication, the switching of light in arrays
of optical waveguides and the propagation of quantized units of magnetic flux in

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4Quantum field theory is not linear per se, but it again depends on the chosen level of de-
tail. The linearity of the individual photon states stems from the property that photons do not
mutually interact. When applied to other interactions, e.g., the electrons, a similar individual
state formulation will give a nonlinear model. The theory is linear when the whole system is
described, but when the many-particle wave function is reduced to many single-particle wavefunc-
tions, describing the occupation of the orbitals of the atoms, the interaction between these must
be taken into account leading to causal loops and nonlinearities. Numerically this means that
the governing equation must be solved self-consistently, as when, e.g., using the Hartree-Fock
method.
Nonlinear localization

Josephson superconducting junctions. The listed phenomena are all examples of nonlinear localization and their emergence as solutions of nonlinear equations is, as we shall see, quite general. Thus, having briefly covered the origin of nonlinearities, the following two sections will instead focus on its effect for the formation and dynamics of nonlinear waves. First we will address solitons, or solitary waves, in continuum systems modelled by partial differential equations and second, nonlinear localization mainly in the form of discrete breathers, or intrinsic localized modes, in discrete systems modelled by coupled ordinary differential equations.

1.1 Solitons

Waves appear in nature in many forms and they can in many instances be accurately modelled by the solution of some partial differential equation. Travelling waves, on the form \( u(x \pm ct) \), are generally associated with the wave equation

\[
\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0,
\]

or its counterpart in more spatial dimensions, that, e.g., can be derived for the vibrations of a string or membrane, the propagation of pressure variations in gases, liquids and solids (sound), the potential or current along a transmission line and the propagation of electromagnetic waves in free space (light). Travelling waves can also be solutions of other linear equations, but unless the temporal and spatial derivatives appear to the same order, as in Eq. (1.1), the form of the wave will not be arbitrary. Instead, travelling waves of a particular form, determined by the equation at hand, can exist while initial conditions having a different form will necessarily disperse (of diffuse). Take, e.g., the diffusion or heat equation,

\[
\frac{\partial u}{\partial t} - \kappa \frac{\partial^2 u}{\partial x^2} = 0,
\]

which has a travelling wave solution on the form \( u(x, t) = Ae^{-a(x-\alpha t)} + B \). This is an unphysical solution\(^5\) and any initial condition deviating from this form will smear out, which is the general characteristic of diffusion\(^6\). Although many equations do have particular travelling wave solutions they do not generally possess some properties associated with many waves in nature, such as localization, i.e., that the energy density of the wave is mainly located in a limited area and decays outside this area. Thus, from linear models we should only expect the propagation of localized waves in models built on proper wave equations, where travelling solutions of any form are permitted. This will change with nonlinear models, since nonlinearities can counterbalance the effect of dispersion or diffusion. The introduction of nonlinear terms in our equation may come from a desire to incorporate

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\(^5\)For a heat conduction problem \( u \) is the temperature and realising this solution on a semi-infinite rod would require an exponential increase of the temperature at the boundary \( (x = 0) \).

\(^6\)The general solution of Eq. (1.2) on the whole real line with initial condition \( u_0(x) \) at \( t = 0 \) is given by \( u(x, t) = 1/\sqrt{4\pi \kappa t} \int_{-\infty}^{\infty} e^{-\frac{(x-y)^2}{4\kappa t}} u_0(y) \, dy \) [190]. From the properties of the convolution integral we can conclude that any initial datum will be smeared.
some process containing a feedback loop, like that for the polaron. If this feedback is positive, the nonlinear terms will work towards self-localization. When nonlinearity and dispersion balance, the result is a localized wave as a solution to our equation. Localized travelling waves therefore appear on a more general basis in nonlinear models than in linear. Moreover, a nonlinear wave cannot be decomposed into smaller fragments in the same way as a linear wave that obeys the principle of superposition. Instead the nonlinear wave must be viewed as an entity in itself, called a soliton or solitary wave, and we should expect the interaction of these waves to be fundamentally different from those of linear ones.

Historically, the first documented observation of a soliton was made by the Scottish engineer John Scott Russell in the Union Canal near Edinburgh who gave the following account of his sighting:

I was observing the motion of a boat which was rapidly drawn along a narrow channel by a pair of horses, when the boat suddenly stopped - not so the mass of water in the channel which it had put in motion; it accumulated round the prow of the vessel in a state of violent agitation, then suddenly leaving it behind rolled forward with great velocity, assuming the form of a large solitary elevation, a rounded, smooth and well-defined heap of water, which continued its course along the channel apparently without change of form or diminution of speed. I followed it on horseback, and overtook it still rolling on at a rate of some eight or nine miles an hour, preserving its original figure some thirty feet long and a foot to a foot and a half in height. Its height gradually diminished, and after a chase of one or two miles I lost it in the windings of the channel. Such in the month of August 1834, was my first chance interview with that singular and beautiful phenomenon which I have called the Wave of Translation...

Russell followed his observation with extensive experiments in water tanks to further determine the characteristics of this special wave and he was able to derive a number of its properties. Interestingly this new understanding led Russell to make significant advances in ship engineering. The solitary wave contradicted the theory of shallow water waves of that time, which predicted that finite amplitude waves could not propagate without change of shape. Subsequently a new theory was presented by Diedrik Korteweg and Hendrick de Vries in 1895, containing the equation (here in normalized units)

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0. \]  

(1.3)

This equation, known as the Korteweg-de Vries (KdV) equation, has, among others, the solution

\[ u(x, t) = 12a^2 \text{sech}^2 \left[ a(x - 4a^2t) \right], \]  

(1.4)

\footnote{A recreation of Russell’s observations on the Union canal can be found at http://www.ma.hw.ac.uk/solitons/press.html.}
Nonlinear localization

Figure 1.1. A two-soliton collision of the KdV equation (1.3), where a high-amplitude fast soliton overtakes a low-amplitude slow soliton. Note that the solitons are phase shifted after the collision.

which accounts for the solitary wave observed by Russell. The term soliton was coined by N.J. Zabusky and M.D. Kruskal in 1965 to emphasize the particle-like properties observed in collisions of the solitary waves (1.4) under numerical simulations of Eq. (1.3) [205]. An example of a collision is given in Fig. 1.1. This property of the KdV-solitons, that they emerge unaltered from collisions, is to be expected for a linear system but is very remarkable when the interactions are nonlinear. An indication that the interaction in fact is nonlinear is that the solitons appear phase shifted after the collision, i.e., they are not in the positions expected if the interactions were linear. This is not a generic property of nonlinear waves, but is conditioned on the KdV equation belonging to the special class of integrable equations that will be further discussed in section 1.1.2.

1.1.1 Dispersion vs. nonlinearity

The route to localization in nonlinear continuum models is that nonlinearity can balance the effects of dispersion, diffraction or diffusion, which act to spread any localized wave form. As the nonlinearity generally represents a self-interaction it will act to contract a wave. We let the KdV equation (1.3) serve as an example.

Ignoring the nonlinearity and investigating the linear dispersive equation

$$\frac{\partial u}{\partial t} + \frac{\partial^3 u}{\partial x^3} = 0, \tag{1.5}$$

we can make use of the principle of superposition and break down the evolution of an arbitrary wave to the evolution of its components. The simplest propagating solution is a plane wave $u(x,t) = e^{i(kx-\omega t)}$, where the frequency and the wave number fulfill the dispersion relation $\omega = -k^3$. The general solution to Eq. (1.5) is given
by the wave packet

\[ u(x,t) = \int_{-\infty}^{\infty} u_k e^{i(\omega_k - \omega(k)t)k} dk \],

(1.6)

where the Fourier coefficients, or plane wave amplitudes, \( u_k \), are determined from initial conditions. Since each component of the wave packet travels at a different phase velocity, \( v_p = \omega/k = -k^2 \), the wave will spread out, or disperse. The dispersion coefficient of a system, defined as \( D = \partial^2/\partial k^2 \), measures how well a wave packet, like Eq. (1.6), will keep its shape during propagation. A zero dispersion means that the wave will be a true travelling wave, like the solutions for the wave equation (1.1). Put another way, when speaking of dispersion we usually mean the relation between frequency \( \omega \) and wave number \( k \) for some travelling plane wave, and this gives us a view of how the temporal derivatives (\( \partial/\partial t \)) are related to the spatial derivatives (\( \partial/\partial x \)). This tells us how the time rate of change of an excitation depends on the slope of the excitation in a particular point. Only if \( \omega \propto k \) the equation is dispersionless, or more transparently, only if the rate of change over time is the same as the rate of change in space the wave will keep its form during propagation. In a linear system a wave packet will propagate with the group velocity \( v_g = \partial \omega/\partial k \), i.e., this is the velocity of the wave packet as a whole and also the velocity at which information can be transmitted. If the group velocity depends on the wave number \( k \), the wave packet cannot move collectively without changing its shape.

With the nonlinearity alone, i.e., ignoring the dispersive term such that

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0, \]

(1.7)
a travelling wave \( u(x,t) = \tilde{u}(x - vt) \) must have an amplitude proportional to the velocity \( v \propto \tilde{u} \). Different points of a wave profile will hence propagate at different velocities, with points of higher amplitude overtaking points of lower amplitude leading to steepening of the wave form.

Any propagating solution of the full equation (1.3) will thus be the subject of two competing processes - the nonlinearly induced wave steepening, or compression, and the dispersive spreading. The wave shape for which these effects are in exact balance is given by Eq. (1.4). Note that the single arbitrary parameter \( a \) affects velocity and amplitude as well as the width of the wave, which highlights how the characteristics of the wave are kept in balance with each other.

### 1.1.2 Integrability

In a nonlinear model we would expect the interaction of waves to be quite complex. The elastic collision of solitons, nearly resembling a linear superposition (see Fig. 1.1), discovered for the KdV equation (1.3) is therefore very remarkable. It is believed that the property of solitons to keep their form in collisions is connected to the existence of an infinite number of conservation laws. A conservation law
can be written on the form of a continuity equation

\[ \frac{\partial I}{\partial t} + \frac{\partial J}{\partial x} = 0. \]  

(1.8)

where \( I \) and \( J \) are functions only of \( x, t \) and \( \partial^n u/\partial x^n \) \((n \in \mathbb{N})\). If the flux, or current density, is such that \( J \to \text{constant} \) when \( |x| \to \infty \), or if periodic boundary conditions are employed, the quantity

\[ I = \int I \, dx \]  

(1.9)

is a conserved quantity during the evolution of the partial differential equation. Solitons can maintain their identities in collisions because of the many constraints imposed on the dynamics by these constants of motion \([127]\). Due to the correspondence with the solvability of finite Hamiltonian systems with as many degrees of freedom as constants of motion \([59, 87]\), partial differential equations with an infinite set of conserved quantities are called integrable\(^8\).

Apart from the KdV equation, other prominent examples of integrable equations are the sine-Gordon (sG) equation

\[ \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + \sin u = 0, \]  

(1.10)

and the nonlinear Schrödinger (NLS) equation

\[ i \frac{\partial \Psi}{\partial t} = \frac{\partial^2 \Psi}{\partial x^2} + |\Psi|^2 \Psi. \]  

(1.11)

These three equations have a number of interesting applications and vouch for the importance of the special property of integrability. The real treat about these integrable equations, and what makes them so interesting, is that they can be completely solved by the method of inverse scattering. This method was first used in 1967 to solve the KdV equation \([86]\). The solution of the initial value problem can be decomposed into a series of linear problems by establishing the equivalence between the evolution equation and an auxiliary scattering problem. In essence, the solution of the evolution equation is the potential in the scattering problem, with solitons corresponding to bound states. The initial value problem is solved by computing the scattering data, i.e., the reflection and transmission coefficients, of the initial condition \((t = 0)\) at infinity. In this asymptotic limit the evolution of the scattering data with time is a simple problem. In fact, the whole idea of the method is that the problem will be linear in the scattering data. With the scattering data at \( t > 0 \) the inverse scattering problem is solved thus obtaining the potential, or solution of the evolution equation for \( t > 0 \). For a linear equation this method reduces to the Fourier transform method. The method of inverse

\(^8\)To be more precise, the term integrable is used for nonlinear partial differential equations that can be solved exactly, by which we mean that the evolution of arbitrary initial data can be expressed analytically. For important classes of equations, the mathematical machinery involved also produces an infinite set of conservation laws.
1.1 Solitons

scattering has since been more generally formulated \[129\] and proven to hold also for the NLS equation \[206, 207\] and the sG equation \[2\]. An excellent account of the details, and the construction of a countable infinite set of conservation laws, can be found in \[182\]. Since analytical tools are available for integrable equations, they are also conveniently used as the starting point of perturbative approaches to other equations \[117\].

Integrability is a nongeneric feature of partial differential equations and almost any perturbation to an integrable equation destroys this feature. In this sense true solitons are structurally unstable and therefore a rare mathematical phenomenon. However, the competing physical processes of nonlinearity and dispersion or diffusion lead to the emergence of localized waves, that in general do not keep their shape in collisions, under rather general circumstances. Therefore physicists often speak of solitons in a less restrictive manner, simply as nonlinear localized waves. We will adopt this nomenclature. Nonetheless, integrable equations have a wide applicability as they in many instances appear as the result of a limiting procedure involving rescalings and an asymptotic, or multiscale, expansion from very large classes of nonlinear evolution equations \[34\]. For example, the KdV equation arises whenever one studies unidirectional propagation of long waves in a dispersive energy conserving medium at the lowest order of nonlinearity and dispersion, and the NLS equation arises in the same context for the study of wave packets \[183\]. In fact, it is possible to obtain a hierarchy of integrable equations by taking multiscale expansions of different orders, i.e., expansions with different time and length scales \[34\]. Thus, expanding beyond the lowest order linear dispersive terms, instead of the NLS equation we may obtain the soliton supporting Hirota equation \[95\]

\[
\begin{align*}
 i \frac{\partial \Psi}{\partial t} &= \frac{\partial^2 \Psi}{\partial x^2} + |\Psi|^2 \Psi + i \frac{\partial^3 \Psi}{\partial x^3} + 3i|\Psi|^3 \frac{\partial \Psi}{\partial x}. \quad (1.12)
\end{align*}
\]

Another higher order integrable equation is

\[
\begin{align*}
 \frac{\partial \Psi}{\partial t} &= \frac{\partial^2 \Psi}{\partial x^2} + |\Psi|^2 + 2\gamma \frac{\partial^4 \Psi}{\partial x^4} + 3\gamma |\Psi|^4 + \gamma \left( 2\Psi \frac{\partial^2 |\Psi|^2}{\partial x^2} + 3 \Psi^* \frac{\partial^2 \Psi^2}{\partial x^2} \right) \quad (1.13)
\end{align*}
\]

where $\gamma$ is an arbitrary parameter \[166\]. Note that Eq. (1.13) reduces to the NLS equation (1.11) for $\gamma = 0$. Thus the balance between nonlinearity and dispersion

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9. Also other mathematical tools are available for equations that are integrable by the inverse scattering transform, such as the Bäcklund transformation (see \[182\]) and the existence of bi-Hamiltonian structure \[135\]. There are also other classes of integrable equations that are exactly solvable by making a change of variables to a linear partial differential equation. A linear equation trivially has a non-countable infinite set of conserved quantities if the dispersion relation is real, namely the magnitude of the Fourier coefficients ($|u_k(t)| = |u_k(0)e^{-i\omega_k t}| = |u_k(0)|$). Since the latter is related to an integral transform, and also since the change of variables generally is non-local, this means that the conservation laws for the nonlinear equation generally also are non-local, i.e., they cannot be expressed on the form of Eq. (1.8).

10. Interestingly, the limiting equation will generally be integrable if any of the equations from which it can be obtained is integrable. This is because the multiscale expansion in general will conserve integrability. Since the limiting procedure is very general and gives the same equation for a very large class of equations, the resulting equation is not unlikely to be integrable. \[34\]

11. The signs of the different nonlinear terms will depend on the form of the equations from which it is derived.
is here carried to the higher order terms, where fourth-order linear dispersion is balanced by a quintic nonlinearity and cubic nonlinear dispersive terms, resulting in the soliton solution,

\[
\Psi(x, t) = \sqrt{2a} \text{sech}[ax - 2abt - 8\gamma(a^2 - b^2)abt] \\
\times \exp \{ -i[bx + (a^2 - b^2)t + 2\gamma(a^4 + b^4)t - 12\gamma a^2 b^2 t] \}.
\] (1.14)

Integrable equations in two spatial dimensions are even rarer than in one dimension, but some examples can be found in [34, 127].

1.1.3 Exotic solitons

In the derivation of many models there is included a balancing between the physical processes involved in the phenomenon we try to model. The KdV equation (1.3), e.g., which models the propagation of waves in shallow water, is valid when the amplitude of the wave is much smaller, and the extent of the wave much larger, than the depth of the water. In this regime the dispersive term and the nonlinear term will be of the same strength. So it is really no surprise that this equation can support solitons, since the exact balancing of dispersion and nonlinearity is inherent in the model. A similar reasoning applies to most integrable equations, as they can be obtained from multiscale expansions of large classes of nonlinear evolution equations. In such expansions, over various time and length scales, terms of equal order in the expansion parameter are collected and this will inevitably lead to dispersive and nonlinear terms that are of the same strength in the range where the expansion is valid. Note, e.g., the higher order terms in Eqs. (1.12) and (1.13), as compared to the NLS equation (1.11). Seen from another perspective: we know that dispersion and nonlinearity are important effects for the propagation of waves and hence we include these in our models. But, simply doing so usually means they appear on equal footing, i.e., we have a first order (linear) dispersive term and a first order nonlinear term, as in the KdV or NLS equations. Assuming that the terms balance we are led to the regime where the equation is valid. By relaxing the ordering of the terms we can derive models that incorporate higher-order dispersion, higher-order nonlinear terms or nonlinear dispersive terms [172, 173], to account for situations when one effect may dominate over the others. In the case of waves in shallow water: if the nonlinearity is dominating over the linear dispersion the wave will steepen. But this will also mean that effects that previously have been neglected may now become important, like higher-order linear dispersion or nonlinear dispersion since the strength of such terms depend on the spatial variation of the wave. Such a model would, e.g., be valid for waves approaching a shoreline where the amplitude of the wave can be much larger than the depth of the water. When the nonlinearity completely dominates over the dispersion the wave will steepen until it breaks, a phenomenon observable along any beach. Hence, relaxing the usual balance of the terms is necessary to capture the dynamics of water waves in some instances. The aim of this section is to discuss some effects in models where nonlinear dispersion plays an important role. The presence of such terms can alter the behaviour of a system drastically. This is illustrated by the following examples.
1.1 Solitons

An integrable extension of the KdV equation \[\text{(1.3)}\] for the propagation of waves in shallow water, including nonlinear dispersive terms, was derived in [35],

\[
\frac{\partial u}{\partial t} - \frac{\partial^3 u}{\partial x^3} + 3u \frac{\partial u}{\partial x} - 2 \frac{\partial^2 u}{\partial x^2} - u \frac{\partial^3 u}{\partial x^3} = 0. \tag{1.15}
\]

This equation has the interesting propagating wave solution

\[u(x,t) = a e^{-|x-\alpha t|}, \tag{1.16}\]

which proves to be stable [130] and of as much fundamental nature as the soliton of the KdV equation [35]. The bell-shaped soliton \[(1.4)\] is replaced by a peaked wave (peakon) that has a finite discontinuity in first derivative at the peak.

For studying the effects of nonlinear dispersion, the equation

\[
\frac{\partial u}{\partial t} + \frac{\partial (u^2)}{\partial x} + \frac{\partial^3 (u^2)}{\partial x^3} = 0, \tag{1.17}
\]

was introduced by P. Rosenau in 1993 [171]. Remarkably, this equation supports solutions that are strictly zero outside an interval,

\[u(x,t) = \frac{4a}{3} \cos^2[(x-\alpha t)/4], \quad |x-\alpha t| \leq 2\pi, \tag{1.18}\]

and which exhibit near elastic collisions similar to the soliton interactions in integrable systems [3]. Because of this resemblance these compact solutions are generally called compactons. Such solutions had also been found earlier in magnetic systems by A.M. Kosevich et al. [120, 121].

The novel feature of the nonlinear dispersion is that the total dispersion of the system will depend on the amplitude of the excitation. As discussed in Sec. 1.1.1, the dispersion relation for an equation relates the variation in time, or frequency \(\omega\), with the variation in space, the wave number \(k\). With nonlinear dispersion, we have besides the dependence on curvature, also a dependence on amplitude. If, for a particular amplitude, the frequency \(\omega\) is independent of the wave number \(k\), as can happen when the dispersion is nonlinear, the rate of change over time of the excitation will be independent of the spatial variation at that point. As a consequence we can allow for arbitrarily large wave numbers, i.e., discontinuous spatial derivatives, at such a point. For Eq. (1.17) this will happen for a zero amplitude and the compacton (1.13) can be joined with the trivial background solution \(u(x,t) = 0\), but at the cost of a discontinuous second derivative at the edge. It is interesting to note that compactons with a zero background cannot form in the presence of linear dispersion, as this implies a term independent of amplitude in the dispersion relation. Generally, solutions with a discontinuity are called nonanalytic or exotic solitons, and have been found in a variety of forms and contexts (e.g. [60, 122, 123, 173]). Some examples are shown in figure 1 in paper II. Nonlinear dispersion is not a sufficient condition for exotic solitons, since it is also required that \(\omega\) can become independent of \(k\). Nor is it a necessary condition, since exotic solitons can form in systems with nonlocal dispersion and nonlinearity [35]. However, the combination of these will effectively lead to a nonlinear dispersion as is explained in paper II.

\[\text{Eq. (1.17) is not integrable and has only four conservation laws.}\]
1.2 Discrete breathers

As discussed in Sec. 1.1, travelling localized solutions quite generally exist in continuum systems as a result of the competition between nonlinearity and dispersion. In a discrete system the effect of nonlinearities can still be self-localization, but since the continuous translational symmetry is broken, a localized excitation is generally more prone to being stationary than moving. To investigate some of the properties of spatially discrete systems we use a model with a lattice of coupled oscillators. Consider for example a one-dimensional chain, as in Fig. 1.2, with identical unit mass oscillators on each site. Assuming coupling only to nearest neighbours, the Hamiltonian, or energy, of the system is

\[ H = \sum_m \left[ \frac{1}{2} p_m^2 + V(u_m) + W(u_{m+1} - u_m) \right], \]  

(1.19)

where \( u_m \) is the displacement from equilibrium, \( p_m = du_m/dt \) the (conjugated) momentum, \( V \) the on-site potential and \( W \) a potential for the coupling. With \( W(x) = x^2/2 \) this is called a discrete Klein-Gordon (KG) model, while for \( V(x) = 0 \) and \( W(x) \) non-quadratic the system is commonly referred to as a Fermi-Pasta-Ulam (FPU) chain. From the Hamilton equations of motion,

\[ \frac{du_m}{dt} = \frac{\partial H}{\partial p_m}, \quad \frac{dp_m}{dt} = -\frac{\partial H}{\partial u_m}, \]  

(1.20)

the dynamical equations are

\[ \frac{d^2 u_m}{dt^2} = -V'(u_m) + W'(u_{m+1} - u_m) - W'(u_m - u_{m-1}). \]  

(1.21)

For small amplitudes we can make a Taylor series expansion of the potentials and keep only the lowest order terms to get the linearized equation

\[ \frac{d^2 u_m}{dt^2} = -V''(0)u_m + W''(0)[u_{m+1} - 2u_m + u_{m-1}]. \]  

(1.22)

Figure 1.2. A chain of coupled oscillators moving in a potential \( V \) coupled by springs described by the potential \( W \).
1.2 Discrete breathers

For the special case $V(x) \sim W(x) \sim x^2/2$ this is the exact equation, which describes a system of coupled harmonic oscillators. The solutions of such a system can all be decomposed into a superposition of normal modes, i.e., plane waves, or phonons, on the form $u_m(t) = \text{Re}\{Ae^{i(\omega_m t)}\}$ with the dispersion relation

$$\omega^2 = V''(0) + 4W''(0) \sin^2 k/2.$$  \hfill (1.23)

Collective motion of the lattice is allowed if the oscillation falls within the set of natural frequencies, the phonon spectrum, determined by Eq. (1.23). One of the most important differences between continuum and discrete systems is that the set of natural frequencies is bounded for a discrete system and forms bands, see Fig. 1.3, while it generally is unbounded for a continuous system. Note also that the width of the bands are proportional to the strength of the coupling $(W''(0))$ between the sites of the lattice.

On a historical note the modern development of nonlinear dynamics was initiated in 1955 by the work of E. Fermi, J. Pasta and S. Ulam, who proposed the model (1.19), with $V(x) = 0$ and $W(x) = x^2/2 + \beta x^3/3$ ($\beta \ll 1$), to study the thermalization of a solid \[73\]. They had access to one of the very first computers, the MANIAC\[13\], and considered this to be a suitable problem for investigation. Up until that time computers had been used exclusively for number crunching and integration, so this was in fact the first ever numerical experiment and the birth of computer simulations as a tool for physicists (see \[54\] for some interesting remarks). Contrary to expectations they observed the recurrence of an initial condition (a single normal mode of the system was excited) after some time when the system seemingly approached thermal equilibrium and the equipartition of energy predicted by statistical physics. The discrepancy between expectations and numerical results was due to a linearized thinking of physical models, often leading to an

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\[13\] The Mathematical Analyzer, Numerical Integrator And Computer that was built for the Manhattan project in 1952 and used for the development of the first hydrogen bomb, ‘Mike’.
Nonlinear localization

analysis of a system based on the properties of normal modes. Thus the evolution
was considered in Fourier space and the effect of the weak nonlinearity was added
as an interaction, or mixing, between the linear modes, i.e., conceptually cause
and effect of the nonlinearity was separated. This discovery led N.J. Zabusky
and M.D. Kruskal to investigate the KdV equation \( \text{(1.3)} \), which after transfor-
mations and rescalings can be obtained as a continuum limit of the FPU chain and is valid
for excitations that are wide compared to the lattice spacing \( \text{(204, 205)} \). They
found, looking at the dynamics as a function of the space coordinates, that the
initial condition broke up into a train of solitons, with varying heights and speeds,
that could pass through each other and after some time reconvene in a wave form
nearly identical to the initial condition. Thus, the existence of solitons could ac-
count for the recurrence of the initial condition in a finite system. These findings
came to have a great impact on the further development and establishment of
nonlinear science as it clearly showed that nonlinear models led to completely new
phenomena \( \text{(183)} \).

The established correspondence between recurrence and an integrable contin-
uum limit \( \text{(14)} \) is related to the behavior of solitons that are large compared to the
lattice spacing. In the following sections we will be concerned with the discrete
nature of the lattice and how nonlinearities can lead to localization also in this
context.

1.2.1 Linear localization

The uniform lattice depicted in Fig. \( \text{(1.2)} \) has a discrete translational symmetry. As
for any physical system we expect this symmetry in some way to be reflected in
the solutions of the corresponding dynamical equations. For linear systems this is
true. The Bloch theorem, drawing on the principle of superposition, tells us that
all normal modes (eigensolutions) are periodic in space \( \text{(15)} \). Since any solution can
be expressed as the superposition of normal modes, this implies that there can be
no localized solutions in a uniform linear lattice \( \text{(16)} \).

If the translational symmetry is broken, so the lattice is no longer periodic,
there can be localized normal modes. This is achieved by adding an impurity to
the lattice, e.g., by having a unit with a different mass, moving in a different on-

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\( \text{(14)} \) If the lattice itself is integrable, recurrence of initial conditions will also occur. The key
feature is that the initial condition during evolution is decomposed into a train of waves that
propagate through the system without disruption. The recurrence time will depend on the time
it takes for each of these waves to propagate through the entire system, which must be finite and
have periodic (or reflecting) boundary conditions.

\( \text{(15)} \) The theorem states that if the lattice, and the corresponding dynamical equations, are in-
variant under a spatial translation, \( r \mapsto r + R \), the normal modes are periodic up to a phase
factor, \( u(r + R) = u(r)e^{ikR} \text{(13)} \). For the one-dimensional chain Eq. \( \text{(1.22)} \) the period is one
lattice unit and any normal mode must fulfill the relation \( u_{m+1} = u_m e^{ik} \) (where the real parts
constitute the physically relevant quantity). For a finite lattice of size \( M \) with periodic boundary
conditions, \( u_{M+1} = u_1 \), the wave numbers are given by \( k = 2\pi n/M, n = 0, 1, \ldots, M - 1 \).

\( \text{(16)} \) If the normal modes are periodic also in time, which is generally the case (and obvious for
Eq. \( \text{(1.22)} \) from an ansatz with separation of variables), an initially localized excitation will in
a finite system recur with a period that is commensurate with the periods of all normal modes
that constitute the excitation. Since solitons can play a similar role in nonlinear lattices, they
are by this correspondence sometimes regarded as a kind of 'nonlinear normal modes'.
1.2 Discrete breathers

Site potential or with a different coupling to neighbouring units. If the difference is large enough, this will give a normal mode localized around the impurity and split-off in frequency from the band of extended normal modes, which corresponds to the phonon spectrum of the uniform lattice. For two or more impurities the number of localized modes depends on the impurities and the model. However, disregarding the details, an impurity-induced localized normal mode will form if it is sufficiently shifted in frequency to lie outside the band of extended modes \[^61\]. The localization can be understood by considering the lattice of coupled oscillators. A transfer of motion between oscillators is facilitated by a mutual coupling and is opposed if there is a mismatch of the individual eigenfrequencies, i.e., the motion is transferred if there is a close resonance between neighbouring oscillators. With an impurity, the frequency mismatch can result in energy being trapped in the oscillation of the impurity site.

If a very large (infinite) number of impurities is added, the lattice will consist of different dynamical units that are random or aperiodically ordered. In a lattice with oscillators of random individual frequencies, it is not difficult to imagine that a wave propagating in such a medium will find regions of large frequency mismatch. A wave surrounded by such regions will be confined to a finite region, and as such be localized \[^61\]. That randomness could lead to localized normal modes was described by P.W. Anderson \[^11\], and is hence called Anderson localization. Quite generally, all normal modes will be localized in one-dimensional \[^152\] and two-dimensional random systems, but at higher dimensionality there may also be extended normal modes \[^61\]. The details depend, e.g., on whether the randomness is in the on-site potential or in the coupling.

The localization in a linear system is connected to the nature and to the positions of the impurities. Compared to a uniform linear lattice, translational invariance is broken, but the principle of superposition is preserved. In a nonlinear lattice the situation is the opposite.

1.2.2 Nonlinear localization

If an oscillator in a linear lattice is periodically forced at a frequency outside the phonon spectrum, the response from the rest of the lattice will be bounded since there are no normal modes at that frequency to put the entire lattice into motion. The response is non-resonant, or similarly, there is a frequency mismatch between the forced oscillator and the natural frequencies of the neighbouring sites preventing a complete transfer of motion. The same is true for small forcing even if the system is nonlinear, i.e., the response is bounded if the frequency is outside the linear phonon spectrum. Of course, for the nonlinear system there is the possibility of exciting nonlinear phonons, i.e., plane waves that are solutions of Eq. (1.21) with an amplitude dependent dispersion relation, but the interactions between a localized disturbance and nonlinear phonons are limited. To induce a nonlinear phonon the entire lattice must be excited with a given amplitude, meaning that there is an energy threshold for such interactions. Hence, it is the interaction with linear plane waves, or rather nonlinear plane waves with small amplitude, that is important.
In a nonlinear system, the frequency of an oscillator will vary with the amplitude, called anharmonic oscillation. If the variation is sufficiently large, the frequency can escape from the phonon spectrum. Provided also that all multiples of the frequency, generated by the nonlinearities, are outside the phonon spectrum, the forcing from that oscillator will cause only a non-resonant response from the rest of the lattice. For weak coupling we can expect that the reaction from the lattice can be taken into account by a slight modification of the motion of the oscillator, and hence the formation of a self-consistent spatially localized time-periodic excitation is possible.

In contrast to Anderson localization and impurity-induced localization, the nonlinear localization is independent of whether the linear modes are themselves localized. If we study the system in the presence of a nonlinear lattice excitation, we can draw some parallels to impurity-induced localization. In both cases it is essential to avoid resonances with the phonon spectrum to prevent that energy is transported away from the bounded excitation. An important difference, however, is that since the nonlinear lattice preserves the translational symmetry a localized excitation may form on any site of the lattice, in contrast to impurity-induced localization where the excitation is bound to the impurity. But if the nonlinear lattice is linearized around the bounded excitation, i.e., we study the evolution of small deviations from the excitation at a given time, this will give a linear system with broken translational symmetry and hence also the possibility for localized normal modes. The nonlinear excitation will act as an impurity. So, just as with an impurity, the evolution of the nonlinear system can be described by localized linear responses, although these responses will affect the system itself and not only the solution. Thus, on a basic level the two processes of localization share common traits, but with the important difference that the nonlinear process has an entangled relation between cause and effect. In essence there is a balance between two effects. The nonlinearity can lead to self-focusing but due to the anharmonicity this gives an increasing frequency mismatch between the coupled individual oscillators, which counteracts further transfer of energy to or from the highly excited sites of the lattice. We therefore refer to nonlinear lattice excitations as intrinsic localized modes. Another commonly used name is discrete breather (DB), first used by D.K. Campbell and M. Peyrard to describe numerically observed discrete analogues of the bound state of the sG equation (1.10) called a breather due to its oscillating behaviour [37]. For an introduction to the theory of DBs see [14, 36, 79].

The existence of discrete breathers in Hamiltonian systems, subject to a non-resonance condition with linear phonons and an anharmonicity condition, has been

\[ u(x, t) = 4 \arctan \frac{\sqrt{1 - a^2 \sin at}}{a \cosh(\sqrt{1 - a^2} x)} \]

for the sG equation (1.10) is a bound state that can be seen as the result of two nonlinear waves propagating in opposite directions [2], like a nonlinear analogue of standing waves on an elastic string. The reason that the breather, which has harmonics \(na\), \(n \in \mathbb{Z}_+\), inside the phonon spectrum \(\omega^2 = k^2 + 1\), can survive resonances is that the infinite number of conservation laws of the sine-Gordon equation puts restrictions on the dynamics [37].
1.2 Discrete breathers

Figure 1.4. Spatial profiles of the most fundamental time-periodic lattice solutions. (a) and (b): one-site, or site-centred, DB. (c) and (d): symmetric two-site or bond-centred DB. (e) and (f): anti-symmetric two-site or bond-centred DB. The excitations in the top row are unstaggered and are expected to appear at frequencies below the phonon band, while the staggered excitations in the bottom row should appear above the phonon band.

rigorously proven by R.S MacKay and S. Aubry [133] and extended to more general systems in [185]. Further, the localization is exponential in the case of nearest-neighbour coupling or exponentially decaying coupling [18] and algebraic in the case of algebraically decaying coupling [19]. The existence proofs are based on a special parameter limit of the studied equations, the anti-continuous limit, where the dynamics of the oscillators are decoupled from each other. In this uncoupled limit, corresponding to $W(x) = 0$ in Eq. (1.19) (KG model), the system consists of independent anharmonic oscillators and a localized solution is easily constructed by putting a single oscillator into motion and leaving all others at rest. By virtue of the implicit function theorem it follows that the localization persists when the coupling is turned on. In principle, we can construct many different types of modes by choosing different configurations in the anti-continuous limit, and further use this configuration for a classification of the modes when the coupling is turned on. The most fundamental mode is obtained with one excited site in the uncoupled limit, and is generally referred to as a one-site or site-centred mode. Similarly, with two neighbouring sites excited with the same amplitude we get a two-site or bond-centred mode, which can be either symmetric or anti-symmetric depending on whether the center displacements are in-phase or out-of-phase. Schematic profiles of these modes are shown in Fig. 1.4. The idea of continuation from the uncoupled limit has been turned into efficient numerical schemes to calculate DBs by following paths in parameter space starting from zero coupling [63, 64, 129, 131]. These
numerical results also show that the continuation of the DBs can be taken beyond the weak coupling limit. A brief description of the path-following methods is found in Sec. 1.2.3. Some other numerical methods are described in [77, 79].

Also for systems with no anti-continuous limit, like the FPU lattice with \(V(x) = 0\) in Eq. (1.19), the existence of DBs has been rigorously proven from a center manifold reduction technique by G. James [98]. See also [76] for a proof for some specific interaction potentials and [17] for a proof based on variational methods. Although there is no uncoupled limit for the FPU lattices the classification of site-centred and bond-centred solutions can still be used.

1.2.3 Stability and numerical methods

Regarding the stability of the nonlinear excitations, it is clear from the generality of the existence proofs that the time-periodic localized solution will be robust to small changes of the governing equations. At least provided that the perturbations conserve the Hamiltonian structure, of which the simplest example is a variation of the parameters of the equation [79]. This is called structural stability. When the perturbation instead is applied to the solution we are concerned with dynamical stability. This form of stability is more direct and probes the immediate neighbourhood of the solution in phase space. It is also very convenient from a numerical point of view. Both forms are of course important since a physical model at best is an approximation of a real situation (structural stability), and since we cannot expect a solution to be exactly reproduced in an experiment (dynamical stability).

For an exact solution the ansatz \(u_m(t) + \epsilon_m(t)\) (and \(p_m(t) + \eta_m(t)\), with \(\eta_m = d\epsilon_m/dt\)) is put into the dynamical equations and the first order terms in \(\epsilon_m(t)\) are kept, leading to a linear evolution equation, depending on the solution \(u_m(t)\), for the perturbation. Taking Eq. (1.21) as an example, the linear stability equation is

\[
\frac{d^2 \epsilon_m}{dt^2} = -V''(u_m)\epsilon_m + W''(u_{m+1} - u_m)(\epsilon_{m+1} - \epsilon_m) - W''(u_m - u_{m-1})(\epsilon_m - \epsilon_{m-1}).
\]

(1.24)

The solution is said to be linearly stable if the perturbation will not grow exponentially. To make this into a more precise statement it is convenient to work with a system of only first order derivatives. Introducing the vector \(u(t) = (\{u_m(t)\}, \{p_m(t)\})\) the system of equations for the coupled lattice can through the Hamiltonian form in Eq. (1.20) be written on the compact form

\[
\frac{du}{dt} = \frac{d}{dt} \begin{pmatrix} \{u_m\} \\ \{p_m\} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \partial H/\partial u_m \\ \partial H/\partial p_m \end{pmatrix} = F(u),
\]

(1.25)

where 0 and I are the zero and identity matrices, respectively. If we also introduce the vector \(\epsilon(t) = (\{\epsilon_m(t)\}, \{\eta_m(t)\})\), the linear evolution equation for a perturbation \(u(t) + \epsilon(t)\) to the exact solution \(u(t)\) is simply

\[
\frac{d\epsilon}{dt} = F'(u)\epsilon.
\]

(1.26)

When the solution, like a DB, is time-periodic, the Jacobian \(F'\) in this equation is also time-periodic. The general method is then to integrate Eq. (1.26) to obtain
the fundamental matrix, or monodromy matrix, $M(t)$ of Eq. (1.24) defined by the mapping

$$
epsilon(t) = M(t)\epsilon(0).$$

(1.27)

The matrix $M(t)$ parametrically depends on $u(t)$ and is periodic with the period $T_b$ of the DB. If the mapping $\epsilon(t)$ is taken to the time $t = T_b$ the Floquet theorem will allow us to reduce the problem of analyzing the perturbations to an eigenvalue problem for $M(T_b)$ [18]. Thus, solving this eigenvalue problem we can conclude that the solution is linearly stable if all eigenvalues have $|\lambda| \leq 1$, i.e., none of the eigenfunctions, which constitute a basis set for any perturbation, will grow exponentially with time. Due to the Hamiltonian nature of the dynamical equations the map (1.27) is symplectic and all eigenvalues, generally called Floquet multipliers, must be on the unit circle for stability since if $\lambda$ is an eigenvalue so are $\lambda^\ast$, $1/\lambda$ and $1/\lambda^\ast$ [170] (see also [14]).

The analysis of stability naturally requires that we know the exact solution to the lattice equations. Only in the rarest cases is it possible to write down the solution explicitly. Hence we resort to numerical solutions of the equations. As described in the previous section, trivial solutions are always known in the anti-continuous, or uncoupled, limit of the equations and other solutions can be obtained by continuation from these solutions. The idea is to use the known solution as an initial condition in a Newton iteration with a slight change of the parameters of the equation. When the iteration has converged, the parameters are again slightly changed and a new solution is found with the previous solution as an initial guess.

Now, suppose that the exact solution of Eq. (1.25) for some fixed set of parameters is $\bar{u}(t)$, and that $u(t)$ is a known vector close to the solution. This means that the system of equations (1.25), by Taylor expansion, approximately can be written as

$$\frac{d\bar{u}}{dt} = F(u) = F(\bar{u}) + F'(u)(\bar{u} - u).$$

(1.28)

If, as assumed, $u(t)$ is close to the solution it will approximately fulfill the evolution equation (1.25), and Eq. (1.28) can be written as $\frac{d}{dt}(u - \bar{u}) = F'(u)(\bar{u} - u)$. This is on the form of the linearized evolution equation (1.29). Since the vector $u(t)$ is known the equation can be straightforwardly integrated to give the fundamental matrix $M(t)$ of the system, and we can write the solution as $u(t) - u(t) = M(t)[u(0) - u(0)]$. Finally, if this is taken to the period $T_b$ of the exact solution, $\bar{u}(T_b) = u(0)$, we are left with

$$u(0) = u(0) + [I - M(T_b)]^{-1}[u(T_b) - u(0)] = G(u).$$

(1.29)

Based on these relations we need to perform a series of calculations to do one iteration in our Newton scheme. Given a vector $u^{(i)}(0)$ of initial data, we first

---

\[18\] The theorem states that if $dx/dt = A(t)x$ with $A(t)$ a continuous $T$-periodic matrix, then the fundamental matrix $M(t)$ of the equation $(dM/dt = AM$ with $M(0) = I$) can be written as a product $M(t) = P(t)e^{\mathcal{B}t}$ where $P(t)$ is $T$-periodic and $\mathcal{B}$ is constant [135]. This means that the eigenfunctions of $A(t)$ are $T$-periodic up to a phase factor, which will correspond to the eigenvalues of $M(T)$.

\[19\] A matrix $M$ is symplectic provided that $M^TJM = J$ for an orthogonal and skew-symmetric matrix $J$, i.e. $J^{-1} = J^T = -J$. 

---
use Eq. \( \text{(1.25)} \) to numerically integrate it to the time \( t = T_b \). We then use this data to integrate Eq. \( \text{(1.26)} \) to obtain the fundamental matrix \( M(T_b) \) defined by \( u^{(1)} \). Finally, the Newton operator \( G \) in Eq. \( \text{(1.26)} \) is used to obtain a new set of initial data \( u^{(i+1)}(0) = G(u^{(i)}) \). This iteration will converge to the fixed point \( \bar{u}(0) = \bar{u}(T_b) \) if the initial guess \( u^{(0)}(0) \) is close to the exact solution. Usually only a few iterations are needed for convergence to sufficient accuracy, unless the matrix \( I - M(T_b) \) is close to singular.\(^2\) Note also that in the process of numerically finding a solution we also obtain the matrix \( M(T_b) \) needed to determine its stability.

In the event that the solution of the dynamical equation is monochromatic, meaning that oscillations in time only occur at the fundamental frequency and that there are no harmonics, i.e., the solution can be written on the form \( \Psi_m(t) = \psi_m e^{-i \Lambda t} \) for constant \( \psi_m \), the eigenvalue problem for the perturbations is considerably simplified as well as the problem of numerically finding solutions. In general there can be no such solutions for systems on the form of Eq. \( \text{(1.21)} \) since the nonlinearities will generate harmonics. But for systems of the discrete nonlinear Schrödinger kind, like Eq. \( \text{(1.38)} \) in Sec. \( \text{1.2.4} \) that are phase invariant this is possible (see further Sec. \( \text{3.2.2} \)). This is also the case of most interest in this thesis. Generally such an equation can be written on the form

\[
\frac{d\Psi_m}{dt} = f(\Psi_m) = f_m, \tag{1.30}
\]

where \( f \) has the property \( f(\{\Psi_m e^{i\phi}\}) = f(\{\Psi_m\}) e^{i\phi}, \phi \in \mathbb{R} \). Since \( \Psi_m \) is complex, Eq. \( \text{(1.30)} \) really represents two coupled real equations. From a numerical point of view it is then convenient to introduce real variables by the substitution \( \Psi_m(t) = [u_m(t) + i v_m(t)] e^{-i M} \). With the vector \( u(t) = \{u_m(t), \{v_m(t)\} \} \), the system of equations are in the rotating frame of reference compactly represented on the form of Eq. \( \text{(1.25)} \).

\[
\frac{du}{dt} = \begin{pmatrix} \{u_m\} \\ \{v_m\} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \{-\Lambda \{u_m\} \} \\ \{v_m \} \end{pmatrix} + \begin{pmatrix} \{\text{Re } f_m\} \\ \{\text{Im } f_m\} \end{pmatrix} = F_\Lambda(u). \tag{1.31}
\]

If we choose the frequency of the frame to be the frequency of the DB solution we are seeking, \( \Lambda = \Lambda_b \), the solution will be stationary. Thus, compared to the more general case we need not perform any time integrations and a much simpler Newton scheme can be constructed. Suppose that \( \bar{u} \) is the exact solution for some set of parameter values of the equation, i.e., \( F_{\Lambda_b}(\bar{u}) = 0 \). If the vector \( u \) is close to the exact solution we have \( F_{\Lambda_b}(\bar{u}) = F_{\Lambda_b}(u) + F'_{\Lambda_b}(u)(\bar{u} - u) \), from which we obtain

\[
\bar{u} = u - [F'_{\Lambda_b}(u)]^{-1} F_{\Lambda_b}(u) \equiv G_{\Lambda_b}(u). \tag{1.32}
\]

\(^2\) For systems with invariance under translations in time (e.g., all Hamiltonian systems), the matrix is always singular. Differentiating Eq. \( \text{(1.25)} \) with respect to time immediately gives that \( \epsilon_0 = du/dt \) is a solution to Eq. \( \text{(1.26)} \) provided that \( u \) is a solution to the dynamical equation. Since \( \epsilon_0 (T_b) = \epsilon_0 (0) \), it is an eigenvector to \( M(T_b) \) with eigenvalue 1, and \( I - M(T_b) \) is singular. A simple trick to solve this problem is to make a restriction to time-reversible solutions, i.e., with \( p_m(0) = d u_m(0)/dt = 0 \). Then one can work in the reduced vector space \( u(t) = \{u_m(t)\} \) and find time-periodic solutions with zero initial velocity. This is often no restriction and will simplify the problem, see also \( \text{[10] [49] [141]} \) for some remarks on the numerical methods.
With the Newton operator $G_{\lambda}$, the iteration $u^{(i+1)} = G_{\lambda}(u^{(i)})$ will converge to the fixed point $\bar{u}$, unless the Jacobian $F'_{\lambda_{b}}$ is close to singular [52].

Having found the solution, linear stability is most simply investigated by applying a perturbation in the rotating frame of reference, where the solution is constant. With the vector $\epsilon(t) = \langle \{\epsilon_m(t)\}, \{\eta_m(t)\} \rangle$ of perturbations, the linearization of Eq. (1.31) is

$$\frac{d\epsilon}{dt} = L\epsilon,$$

where the matrix $L = F'_{\lambda}$ is constant, but depends on $u$. For a Hamiltonian system $L$ is infinitesimally symplectic and will have the simultaneous eigenvalues $\pm \lambda$, $\pm \lambda^*$, i.e., linear stability of the solution is ensured if all eigenvalues lie on the imaginary axis. Note also that due to the phase invariance there will always be a double eigenvalue at the origin.

Since the dynamics of the perturbations are obtained from linearizing around the DB solution, the evolution equations describe a linear system with broken translational symmetry where the localized excitation will act as an impurity. The eigenfunctions, or normal modes, of this system will thus contain a set of extended eigenfunctions corresponding to the linear spectrum of the original dynamical equation. Close to the anti-continuous limit, where the linear spectrum is narrow, and as long as the harmonics of the DB solution lie outside the band of phonon modes, perturbations described by the extended eigenfunctions will not cause instabilities [14, 20]. However, for stronger coupling such instabilities are possible in a finite system [14, 140]. Due to the DB acting as an impurity there will also be some localized modes, a pair of which will only continue the DB solution forward or backward in time [79]. An instability caused by localized eigenfunctions will, at least not initially, destroy the localization but will work to transform the DB into some other configuration. Typically, the DB is transformed to a solution of lower energy, in which radiation through interaction with extended modes is inevitable, or, as will be discussed in Sec. 1.2.6 to a moving excitation.

Quite generally the symmetry of the DB solution is connected to its dynamical stability. The site-centred localized mode, corresponding to a single excited mode for the general equation (with eigenvalue 1 of $M(T_b)$) and the phase mode for the simpler phase invariant equation (with eigenvalue 0).

21 However, the Jacobian will always be singular in the general formulation if the dynamical equation is phase invariant. If $u_{m} + v_{m}$ is a solution so is $(u_{m} + iv_{m})e^{i\phi} = u_{m} + iv_{m} + \phi \cdot (-u_{m} + iv_{m})$, where we have taken $\phi$ to be infinitesimal. On vector form we have that if $u = \{(u_m), \{v_m\}\}$ is a solution, so is $u + \epsilon_0$ for $\epsilon_0 = \phi \cdot \{(u_m), \{v_m\}\}$. Since the solution is constant, Eq. (1.31) becomes $0 = F_{\lambda_{b}}(u + \epsilon_0) = F_{\lambda_{b}}(u) + F'_{\lambda_{b}}(u)\epsilon_0 = F'_{\lambda_{b}}(u)\epsilon_0$. Thus $\epsilon_0$ is an eigenvector with eigenvalue 0 and the Jacobian is singular. This problem can be dealt with by fixing the global phase, e.g., by requiring that $v_k = 0$ for some site $k$ of the lattice. Also, as shown in Sec. [82] it will often suffice to study only real solutions, with $v_m = 0$ for all $m$, and the complexity of the problem is even further reduced (see also [63] [64]).

22 The matrix $L$ is called infinitesimally symplectic provided that $L^T J + JL = 0$ for an orthogonal and skew-symmetric matrix $J$. A necessary and sufficient condition for this is that $L = JS$ with $S$ a symmetric matrix.

23 The condition that must be fulfilled is $n\omega_{b} \neq 2\sqrt{V''(0)}$, where $\omega_{b}$ is the DB frequency and $n \in \mathbb{Z}$.

24 These will simply be the trivial eigenmodes discussed in the footnotes above, i.e., the velocity mode for the general equation (with eigenvalue 1 of $M(T_b)$) and the phase mode for the simpler phase invariant equation (with eigenvalue 0).
a nonlinear KG lattice \[14\], whereas the symmetric bond-centred mode, with two main excited sites, is unstable (see \[79\] and references therein). This will not always be the case when the coupling of the system is increased. For a one-dimensional FPU lattice it is instead the two-site solution that is stable, while the one-site solution is unstable \[178\].

### 1.2.4 Modulational instability

As discussed in Sec. 1.2.2 DBs may exist in a nonlinear system if they oscillate with frequencies outside the linear spectrum, Eq. (1.23). Though we may expect a DB to form from an initial condition where energy is localized, like a non-resonant periodic forcing at some lattice site which is turned off at \( t = 0 \), a more interesting question is if they can form spontaneously from non-localized initial conditions. That would mean that the presence of localized excitations in nonlinear discrete systems, e.g., used as models for crystal lattices and vibrations in organic molecules like DNA, could make important contributions to scattering and transport properties in these systems. Moreover, in a microscopic system it is generally not possible to excite only a few sites, but energy distributed over the entire system can easily be introduced. In this context we are interested in families of DBs that contain solutions that are weakly localized, since these are the ones we expect to initially appear from extended initial conditions. More explicitly we can argue for a connection to plane wave solutions, since in the limit of very weak localization the DB will be nothing but a plane wave with a long-wavelength modulation. The weak localization seems only to be possible if the DB is close to the linear spectrum, i.e., it is only for small amplitude excitations that the frequency of the DB will be close to the frequency of a plane wave and it is only then we will get localized excitations that decay to zero. Thus for a DB solution to exist just outside the linear spectrum it should appear from a (tangent) bifurcation with a band edge linear plane wave that is continued into the nonlinear regime \[79\], i.e., the plane wave must become unstable to a modulation of its wavelength. In this weakly nonlinear, or low-amplitude, regime the modulational instability of plane waves is a necessary condition for the existence of DBs \[79\].

For a simple coupled lattice with a nonlinear on-site potential, i.e., a KG model with \( W(x) = \alpha_2 x^2 / 2 \) and \( V(x) = \omega_0^2 x^2 / 2 - \beta x^4 / 4 \), the dynamical equation (1.21) will take the form

\[
\frac{d^2 u_m}{dt^2} = \alpha_2 (u_{m+1} - 2u_m + u_{m-1}) - \omega_0^2 u_m + \beta u_m^3. \tag{1.34}
\]

The on-site potential \( V(x) \) is quite general as it can be taken as a Taylor series expansion of a more general symmetric potential for small amplitude oscillations around \( x = 0 \)25. The linear spectrum is given by \( \omega^2 = \omega_0^2 + 4\alpha_2 \sin^2 \frac{k}{2} \), for plane waves with wave number \( k \). The fundamental frequency of the individual oscillators is \( \omega_0 \), corresponding to the lower band edge in Fig. 1.3 so if the nonlinearity and the coupling is weak this will approximately be the frequency of oscillation

---

25The requirement of a symmetric potential is not a necessary condition in the following derivation \[113\].
1.2 Discrete breathers of the linear lattice. Thus we can study the motion of the lattice in the rotating-wave approximation, as a modulation of an oscillation at the frequency $\omega_0$. This is described by the ansatz

\[ u_m(t) = \Psi_m(t) e^{-i\omega_0 t} + c.c., \]  

(1.35)

where the envelope $\Psi_m$ is slowly varying in time and modulates the fast oscillation at frequency $\omega_0$. Thinking in terms of oscillators, the rotating wave ansatz simply means that we replace the position–momentum description of the oscillators with a complex rotating amplitude (a phasor), the real and imaginary projections of which correspond to the position and momentum of the oscillator, respectively. Inserting Eq. (1.35) in Eq. (1.34) results in the equation

\[ \frac{d^2 \Psi_m}{dt^2} - 2i\omega_0 \frac{d\Psi_m}{dt} - \alpha_2 (\Psi_{m-1} - 2\Psi_m + \Psi_{m+1}) - 3\beta|\Psi_m|^2 \]  

\[ - \beta \Psi_m^3 e^{-3i\omega_0 t} + c.c. = 0. \]  

(1.36)

Thus, with the approximation of slow variation,

\[ \left| \frac{d\Psi_m}{dt} \right| \ll \omega_0|\Psi_m|, \]  

(1.37)

and disregarding the fast oscillating terms with time-dependence proportional to $3\omega_0$, the envelope of the modulation is described by the discrete nonlinear Schrödinger (DNLS) equation

\[ i \frac{d\Psi_m}{dt} = \tilde{\omega}\Psi_m + C(\Psi_{m-1} + \Psi_{m+1}) + 2\gamma\Psi_m|\Psi_m|^2, \]  

(1.38)

with parameters $\tilde{\omega} = \alpha_2/\omega_0$, $C = -\alpha_2/2\omega_0$ and $\gamma = -3\beta/4\omega_0$. The DNLS equation (1.38) is a generic equation that will arise in contexts where the first effects of coupling and nonlinearity are considered. It is also in many instances a model in its own right, as exemplified in chapter 2. The plane wave $\Psi_m(t) = \sqrt{\rho}e^{-i(\varphi_m + \Lambda t)}$ is a solution if the frequency fulfills the dispersion relation

\[ \Lambda = \tilde{\omega} + 2C \cos \varphi + 2\gamma \rho = \frac{2\alpha_2}{\omega_0} \sin^2 \frac{\varphi}{2} - \frac{3\beta}{2\omega_0} \rho. \]  

(1.39)

In the linear limit ($\gamma = 0$), this will approximate the linear spectrum of the original problem Eq. (1.34) close to the lower band edge $\varphi = 0$ ($k = 0$), where $\omega \approx \Lambda + \omega_0$, and in the weakly nonlinear regime it corresponds to analyzing the behaviour of the dominating first harmonic of a nonlinear plane wave. Note that the nonlinearity in Eq. (1.38) not will generate any higher harmonics. Subjecting the plane wave $u$
to a small perturbing modulation with wave number $q$ its linear stability can be investigated,

$$
\Psi_m(t) = \left[ \sqrt{\rho} + u(t)e^{iqm} + v^*(t)e^{-iqm} \right] e^{-i(\varphi_m + \Lambda t)}. \tag{1.40}
$$

Inserting this perturbed solution in Eq. (1.38) and keeping only terms linear in $u$ and $v$ yields the eigenvalue problem

$$
\frac{d}{dt} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} a + b & c \\ -c & a - b \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \Omega \pm \begin{pmatrix} u \\ v \end{pmatrix}, \tag{1.41}
$$

with $a = 2C \sin \varphi \sin q$, $b = 2C \cos \varphi (\cos q - 1) + 2\gamma \rho$ and $c = 2\gamma \rho$. The plane wave is stable if the eigenfrequencies $\Omega = a \pm \sqrt{b^2 - c^2}$ are real for all $q$, meaning that the modulating perturbation will not grow. Explicitly, the eigenfrequencies are given by

$$
\Omega = 2C \sin \varphi \sin q \pm \sqrt{16C \cos \varphi \sin^2 \frac{q}{2} \left( \cos \varphi \sin^2 \frac{q}{2} - \gamma \rho \right)}. \tag{1.42}
$$

From the expression under the square root we can immediately determine that plane waves at the lower band edge, $\varphi = 0$, will be unstable to long-wavelength modulations, $q \approx 0$, in the nonlinear regime, $\gamma < 0$ (and $C < 0$). In fact, the band edge plane wave will be unstable to all modulations provided that $\rho > C/\gamma = 2\alpha_2/3\beta$.\[119\]

We conclude that under general circumstances localized excitations can emerge from non-localized initial conditions in models on the form of Eq. (1.34), and that their wave profile will be accurately modelled by the DB solutions of Eq. (1.38). The solutions appear below the phonon band and will have a spatial profile as that indicated in the top row of Fig. 1.4. For Eq. (1.34) we can only make predictions for weak coupling ($\omega_0^2 \gg 4\alpha_2$), where the width of the phonon band is small. It is only in this limit that our approximations are valid and we can safely neglect the influence of higher order harmonics. In this limit we can also, in the same formulation as above, investigate the possible bifurcations at the upper band edge, corresponding to $\varphi = \pi$ ($k = \pi$). Since the expression under the square root in Eq. (1.42) will be positive for all values of $q$ for this wave number, the plane wave will be stable. Hence there will be no bifurcation and there can be no stable localized solutions immediately above the phonon band. However, if the sign of the nonlinearity is reversed, so that $\gamma > 0$ ($\beta > 0$ and still $C < 0$), the situation will be exactly the opposite and localized solutions can only exist above the phonon band but not below.\[27\] Since the DB solutions appear from a plane wave with complete out-of-phase oscillations they will have the staggering form depicted in the bottom row of Fig. 1.4. Studying the bifurcation of the plane waves in more detail reveals that a sufficient criterion for a bifurcation to occur is that the frequency of the plane wave is repelled from the linear spectrum when the energy (amplitude) is reversed.

\[27\] Note that the change of sign of the nonlinearity in Eq. (1.38) corresponds to reversing time and making a staggering transformation, i.e., $\Psi_m(t) \rightarrow (-1)^m \Psi_m(-t)e^{-2i\omega t}$. This means that the roles of long and short wavelengths have interchanged, since all wave numbers have been shifted by $\pi$. See also further about anomalous diffraction in Sec. 2.1.5.
1.2 Discrete breathers

increased \([79]\). This is consistent with Eq. \((1.39)\), and can be expected since it is imperative that the localized solution to which the plane wave bifurcates avoids resonances with the linear spectrum.

A similar analysis can be performed for a lattice with a nonlinear coupling instead of a nonlinear on-site potential. Again we can consider a quite general nonlinear coupling on the form

\[
W(x) = \alpha_2 x^2 / 2 + \alpha_4 x^4 / 4
\]

and arrive at the FPU model \((V(x) = 0)\)

\[
\frac{d^2 u_m}{dt^2} = \alpha_2 (u_{m+1} - 2u_m + u_{m-1}) + \alpha_4 [(u_{m+1} - u_m)^3 - (u_m - u_{m-1})^3]. \tag{1.43}
\]

Since we now are strictly interested in the upper band edge \((k = \pi)\) of the linear spectrum, \(\omega^2 = 4\alpha_2 \sin^2 k / 2\), we make a rotating-wave approximation to study the modulations at the frequency \(\omega_c = 2\sqrt{\alpha_2}\). Since the phonons at the upper band edge correspond to complete out-of-phase oscillations of neighbouring sites it is also convenient to introduce a staggering transformation in the ansatz. We set

\[
u_m(t) = (-1)^m \Psi_m(t)e^{-i\omega_c t} + c.c., \tag{1.44}
\]

which under the same approximations as above will lead to a DNLS equation with nonlinear coupling,

\[
\frac{d\Psi}{dt} = \tilde{\omega}\Psi + C(\Psi_{m-1} + \Psi_{m+1}) + \gamma \left[2\Psi_m|\Psi_m|^2 + \Psi_{m-1}|\Psi_{m-1}|^2 + \Psi_{m+1}|\Psi_{m+1}|^2 - 2\Psi_m(\Psi_{m-1}^2 + |\Psi_{m-1}|^2) + \Psi_{m+1}(\Psi_{m+1}^2 + |\Psi_{m+1}|^2) + 2\Psi_m(\Psi_{m-1}^2 + |\Psi_{m-1}|^2) + \Psi_{m+1}(\Psi_{m+1}^2 + |\Psi_{m+1}|^2)\right]. \tag{1.45}
\]

where \(\tilde{\omega} = -\alpha_2 / \omega_c\), \(C = \alpha_2 / 2\omega_c\), and \(\gamma = 3\alpha_4 / 4\omega_c\). \([32, 33, 47]\). Eq. \((1.45)\) will, similar to the on-site DNLS equation \((1.38)\), be a generic model for studying the first effects of nonlinear coupling. The plane wave \(\psi_m(t) = \sqrt{\rho} e^{-i(\varphi_m + \Lambda t)}\) is a solution for \(\Lambda = \hat{\omega} + 2C \cos \varphi + 2\gamma \rho (3 + 4 \cos \varphi + \cos 2\varphi)\). This dispersion relation is an approximation of the linear spectrum of Eq. \((1.43)\), \(\omega \approx \Lambda + \omega_c\), valid near the upper band edge \(k = \pi\), which now corresponds to \(\varphi = 0\) due to the staggering transformation. Adding a modulating perturbation as in Eq. \((1.40)\) we are again led to an eigenvalue problem on the form of Eq. \((1.41)\), where the eigenfrequencies
now are given by

\[ \Omega_{\pm} = 2[C + 4\gamma \rho(1 + \cos \varphi)] \sin \varphi \sin q \pm \left\{ 16[(C + 2\gamma \rho) \cos \varphi + 2\gamma \rho \cos 2\varphi] \sin^2 \frac{q}{2} \right. \\
\left. \times \left[ ((C + 6\gamma \rho) \cos \varphi + 2\gamma \rho(2 + \cos 2\varphi)) \sin^2 \frac{q}{2} - \gamma \rho(3 + 4 \cos \varphi + \cos 2\varphi) \right] \right\}^{1/2} \]

(1.46)

Studying the signs of the expressions under the square root \((C, \gamma > 0)\), we again find that nonlinear plane waves with wave numbers \(\varphi \approx 0\) will be modulationally unstable for perturbations with long wavelength \(q \approx 0\). However, in this case short-wavelength modulations \(q \approx \pi\) will always be stable. Hence DBs can exist with frequencies above the linear spectrum of Eq. (1.43). Also, in the FPU model the plane wave must be repelled from the linear spectrum with increasing energy for a bifurcation to occur, but this is only a necessary, and not a sufficient, condition [79].

In papers III and V, we are interested in the modulational instability, or rather stability, of plane waves for a more general form of Eq. (1.45) in both one and two dimensions. Modulational instability is also discussed for a continuous system in paper II, where it is used to understand the instability of some solitons.

### 1.2.5 Formation, persistence and detection

Though the modulational instability of plane waves predicts the formation of localized excitations it is not certain that they will actually form or persist in a real system. Even if stable DBs exist as solutions to the dynamical equations, the longevity of localized excitations cannot be guaranteed. The analysis of linear stability generally regards the pure excitation and does not take into account the interactions with other excitations that may be present in the lattice, but stability is of course an indication that the localized excitation will be favored over other configurations. Performing long-time simulations of discrete dynamical systems with extended initial conditions will address these issues. Indeed, both for the KG models [163] and the FPU models [30, 53, 61], as well as for the DNLS models [101, 103, 168], the spontaneous creation of localized excitations are observed in numerical simulations with initial conditions ranging from slightly perturbed plane waves to noisy backgrounds corresponding to thermal fluctuations of the lattice. In the initial stages of the evolution, the modulational instability of plane waves leads to the creation of many small-amplitude, or weakly localized, excitations as expected from the analysis above. Beyond this initial stage the modulational instability approach is no longer valid, and we can make no prediction for the formation of large-amplitude excitations. However, as exemplified in Fig. 1.5, the numerics show that the smaller excitations will coalesce into larger localized excitations, and

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The details of the eigenvalue problem can be found in paper III where the derivation is made for a slightly more general form of Eq. (1.45). The same problem for a two-dimensional lattice is solved in paper V. See also [101] for a discussion of modulational instability in a mixed KG-FPU model, i.e., a one-dimensional chain with both a nonlinear on-site potential and nonlinear coupling.
1.2 Discrete breathers

Figure 1.5. The evolution of the energy density in a KG lattice with a noisy plane wave as initial condition. The energy density is given in gray scale with white being zero and black being the maximum value during the simulation. Initially the energy density is very near uniform, then, due to modulational instability, small DBs form. These will collide and large DBs absorb the smaller more mobile DBs, thus growing into larger immobile DBs pinned to the lattice. The figure is adopted from reference [163] by M. Peyrard.

that the latter will feed on the former. Thus the number of localized entities will decrease with time, but the ones remaining will grow as well as the total energy found in these localized oscillations compared to extended (phonon) oscillations. Some details of the interactions and the exchange of energy between localized excitations and phonons can be found in [103, 168]. The remaining large-amplitude DBs can persist for very long times [101, 163], although there are additional interactions that after some time may lead to their decay and destruction [51, 100, 103]. The question whether localized excitations will be present in the final thermalized state of the discrete system, or if the energy will spread evenly in the lattice, is connected to the energy density in the system and its relation to the densities of other conserved quantities [101, 105, 169, 174]. As indicated above, in the latter case there can be a long-lived transition state where localized excitations are present.

The above discussion is more pertinent to systems that are microscopic or smaller, than to macroscopic systems, by which we mean systems where some control can be exercised as to the nature of excitations at specific sites in the lattice. In microscopic systems, typically crystal lattices or biomolecules, the numerical simulations strongly suggest the presence of nonlinear localized excitations.
However, there are difficulties with the direct experimental detection of energy localization in such systems. Vibrational spectroscopy of crystals with photons, infra-red or Raman, have limitations in resolution ($\sim 10^3$–$10^4$ Å). This is obviously beyond the resolution needed to observe spatial vibrations extended over a limited number of sites in a uniform lattice. This follows from the uncertainty principle, $\Delta x \Delta k \sim 1$. To resolve something with a spatial extent of 1 Å the wave number distribution of the wave packet must be at least 1 Å$^{-1}$, which is not possible with photons [74]. Thus, due to the quantum indistinguishability of individual atoms or molecules in a crystal lattice it is not possible to probe the local character of an oscillation. High enough resolution can be achieved with inelastic neutron scattering, but then arises instead the problem of assigning the peaks of the absorption spectra to nonlinear excitations, and not to other localized vibrations due to disorder or impurities [74, 163]. Direct measurements of nonlinear localized oscillations in crystals or extended biomolecules, with an $\alpha$-helix backbone, by standard spectroscopy techniques are therefore somewhat inconclusive (see further comments in [74]). Energy localization in smaller systems like single molecules with a vibration in a specific bond within the molecule, a local mode, can be detected by spectroscopy. The anharmonicity is inferred from a frequency red-shift of the oscillation as the intensity is increased, and this is an indirect proof of localization in these cases [36]. Recent advances, with the development of nonlinear pump-probe spectroscopy by P. Hamm and co-workers (see [93] for an introduction), have made it possible to probe the nonlinear responses of an oscillation only, i.e., a harmonic oscillation will give no response at all. With this technique it has been possible to determine the self-trapped nature of oscillations in crystalline acetanilide (ACN), with serves as a model system for proteins. Still, the response from the pump-probe experiment must be interpreted on a case-to-case basis, since anharmonicity not necessarily implies localization.

From this discussion it is apparent that the observation of nonlinear localization is considerably easier in macroscopic systems, this not barring the importance of the presence of nonlinear localization in microscopic systems. The latter can in many instances be inferred indirectly from the properties of these systems and also from its explicative power for specific phenomena. This includes the role of localized excitations for the energy transport in biomolecules, e.g., with connection to the local opening of the DNA double-helix, or as the seed for conformational changes in a biopolymer [144, 164, 182]. Also, a strong agreement of theoretical and experimental results suggests the existence of localized modes in the charge transfer solid PtCl [72, 192, 200] and could account for the quantized steps in the time-dependent emission spectra from nonlinear spectroscopy of an antiferromagnetic spin lattice [180]. In nonlinear discrete systems where excitations can be visualized in the spatial domain, instead of the Fourier domain as with spectroscopy, the experimental detection of nonlinear localized excitations is indisputable and ubiquitous. Examples are vibrations in micromechanical cantilever arrays [179], the voltage distribution in an electrical lattice [142], the excitation of whirling states in arrays of superconducting Josephson junctions [26, 196], the localization of light in arrays of nonlinear optical waveguides [68] (Sec. 2.1.5) or optically induced waveguides in photorefractive materials [82] and the self-trapping of Bose-
Einstein condensates in a periodic optical potential \[12\] (Sec. 2.2). As much as these examples represent significant technological advances and prospects for interesting applications they are also a playground for nonlinear physics where the theory can be tested. For example, the modulational instability leading to creation of small amplitude nonlinear excitations, as discussed above, can be observed in optical waveguide arrays \[143\] and Bose-Einstein condensates in a periodic potential \[71\]. In conclusion, it is evident that DBs are important for the behaviour of physical systems.

1.2.6 Mobility

In continuous nonlinear systems, localized travelling waves, or solitons, are formed by the balance between nonlinearity and dispersion, as discussed in Sec. 1.1. In a discrete system, the effect of anharmonicity can prevent the spreading of energy from a localized oscillation if it is nonresonant with the rest of the lattice. It is imperative that the frequency of oscillation of the DB is not compatible with the frequency of the individual oscillators in the lattice. The physical process that leads to localization in a lattice with weak coupling is thus relying on the discreteness and the breaking of the continuous translational symmetry as compared to a continuum system. A DB is therefore more prone to being stationary than mobile. For larger coupling we may expect mobility of localized modes. In this limit the excitations are wide, compared to the lattice spacing, and are hence more insensitive to the effects of the lattice discreteness. The excitation is then well described by a continuum approximation and the dynamics is effectively governed by a nonlinear partial differential equation, leading to soliton-like behaviour. These excitations are therefore generally referred to as \textit{discrete envelope solitons}, or \textit{lattice envelope solitons}. For highly localized excitations, with only a few main excited sites, the situation is more intricate, as will be described in the rest of this section.

From numerical simulations it has been shown that large-amplitude localized excitations can propagate in one-dimensional lattices with nonlinear coupling (FPU lattice) \[193, 194\]. However, in two dimensions strongly localized modes remain immobile \[51\]. For the lattices with a nonlinear on-site potential (KG lattice), mobility of highly localized modes is resisted \[22, 55\]. Efforts to understand this trapping, or \textit{pinning}, of the energy to a site in the lattice have been done. In a discrete system there is obviously a difference between a DB centred on a lattice site and a DB centred inbetween lattice sites (see Fig. 1.4). The site-centred DB is generally stable, while the bond-centred DB is unstable, at least for weak coupling in a KG lattice. Since both modes are solutions of the dynamical equations, this means that the site-centred DB will represent a potential minimum on some energy surface and the bond-centred DB will be at a potential maximum (or a saddle point). A travelling DB in the lattice will thus experience a periodic potential. If the travelling DB is not an exact solution, and there are strong indications that there in general are none in KG lattices \[22\] (but see also the discussion below), it will lose some energy to radiation and thus eventually get trapped in one of the potential minima. However, it is possible to find exact localized travelling waves also in KG lattices for some specific potentials. These waves have no oscil-
lating degree of freedom and are therefore not moving DBs, but discrete solitons. The construction of the potentials is made from a reversed engineering approach, given the shape of the travelling wave \[80\]. Exact travelling waves also exist in models that are integrable, perhaps the most important being the Ablowitz-Ladik equation
\[\begin{align*}
i \frac{d \Phi_m}{dt} &= (C + 2\gamma |\Phi_m|^2)(\Phi_{m-1} + \Phi_{m+1}). \tag{1.47}\end{align*}\]
which is a discretization of the NLS equation \[1.11\] that retains the property of integrability \[3, 4\]. It has an exact travelling DB solution \[182\],
\[\Phi_m(t) = \sqrt{\frac{C}{2\gamma}} \sin b \text{sech}(bm - ct) e^{-i(am + \Lambda t)}, \tag{1.48}\]
with \(c = 2C \sin b \sin a\) and \(\Lambda = 2C \cosh b \cos a\) and the free parameters \(a\) and \(b\). Integrability is a rare property for lattice equations.

Due to the oscillating degree of freedom of a DB there is in general no way to quantitatively characterize the periodic potential \[22, 78\], generally known as a Peierls-Nabarro (PN) potential. Since the DBs come in families parameterized by the frequency of oscillation, there are always many solutions of both types with different energies. Thus, if we try to perturb a stable DB to overcome the potential barrier and make it mobile, to which of the unstable DBs should it be compared? The concept of the PN potential does however offer an explanation of the numerically observed pinning. A working definition, to get quantitative estimates, is to consider solutions with the same frequency \[55\], but there is nothing that will guarantee that the frequency of oscillation is constant for a travelling DB. In principle, the PN-barrier will depend on the trajectory the travelling DB follows in phase space and therefore it cannot be unambiguously defined \[78, 79\]. A method to analyze the travelling DBs was suggested in \[134\], where an effective Hamiltonian is introduced for the variables describing the translational motion by averaging over the periodic variables, i.e., the oscillation. This means that the mobility is considered for solutions that have a constant area, or action, in phase space, and the definition of the PN potential will be clear under this constraint. For the KG and FPU lattices approximate dynamics can be obtained by the rotating-wave ansatz, leading to DNLS equations as described in Sec. 1.2.4. By treating Eqs. \[1.38\] and \[1.45\] as perturbed versions of the integrable Ablowitz-Ladik model \[1.47\], an effective dynamics for the travelling waves is obtained. It is concluded that highly localized modes cannot propagate in the KG lattice above a threshold amplitude but it is possible in the FPU lattice in one dimension \[47, 115\].

\[29\] The name comes from the similar problem involving travelling kinks, that have no oscillating degree of freedom and therefore allow for a precise definition of the potential.
stationary site-centred and bond-centred solutions at constant norm will facilitate a meaningful interpretation of the PN-barrier. Indeed for DNLS models a quantitative agreement between the size of the energy difference and the energy supplied to get moving excitations is reported [88, 199]. However, as explained in paper [V] the straightforward interpretation of the PN-barrier is not always this trivial also for some DNLS models. Moreover, as an approximation to the general nonlinear lattices the estimates of the potential can be as much as an order of magnitude off. This is related to the influence of higher-order terms not included in the rotating-wave approximation [22].

The existence of an additional conserved quantity, besides the Hamiltonian, for the DNLS models will allow us to consider specific members of the DB families parameterized by the frequency, the ones with the same norm. Still, the stationary solutions will of course not be on the trajectory in phase space defined by a travelling excitation, but the energy difference will give a lower bound to the energy that needs to be supplied to a stable stationary DB to achieve mobility.

In integrable models, like the Ablowitz-Ladik equation (1.47), the exact travelling solutions also exist for zero velocity ($\alpha = 0$ in Eq. (1.48)). For such models there is hence no PN-barrier, since, with given norm, the Hamiltonian is independent of the position of the DB in the lattice. Numerically it has been demonstrated that when the equations depart from the integrable limit the exact travelling DB solution develops a resonant tail [88]. The amplitude of this tail grows when the equation is farther away from the integrable limit, or alternatively as the size of the PN-barrier increases from zero. It is inferred that the effect of pinning is overcome by a periodic exchange of energy between the localized core and the oscillating tail as the excitation moves through the lattice and the periodic PN potential. This result can also be extended to two dimensions [89]. However, there is a limit as to how far these numerically exact mobile solutions can be continued away from the integrable limit, with broad solutions being more persistent as can be expected [88].

To have good mobility of highly localized modes we should thus look for ways to minimize the PN-barrier. For the cubic DNLS equation (1.38), the difference in Hamiltonian between site-centred and bond-centred DBs is an increasing function of the norm [151]. Going beyond this most simple DNLS model the behaviour is changed. With other types of nonlinearities, like a saturable nonlinearity [92, 199] or nonlinear coupling as in papers [I] and [V] (see also [157]), a vanishing of the energy difference at certain points has been demonstrated. At these points the mobility of highly localized modes is generally very good, but there are exceptions as shown in paper [V]. Away from these points mobility is poor and only propagation of broad localized excitations are allowed over any appreciable distances.

When perturbing a stationary DB to induce mobility the form of the perturbation will naturally be important, and it should contain some velocity component (or imaginary component in the case of complex variables as for the DNLS equa-

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\[30\] This also means that exact travelling localized solutions may exist even if there is an energy difference between stationary modes. An explicit example for kinks is given in [80].

\[31\] There is also a large class of DNLS models that support translationally invariant states. These equations conserve, apart from a norm, also momentum, but they cannot be written on a standard Hamiltonian form [159]. Amongst them is the integrable Ablowitz-Ladik model.
Nonlinear localization

The optimal perturbation to achieve mobility is to kick the solution along a so-called depinning mode \[40\]. Close to a point in parameter space where a fundamental DB changes its stability, the eigenmode yielding the instability will have a form that can tilt the DB in either direction in the lattice. See Fig. 3 in paper I for an example. When the DB is unstable this is the mode that will grow and change the form of the DB. When the DB is stable, perturbing the velocity components of the solution along this mode will break the symmetry. For a sufficiently large perturbation the DB will then be tilted in one direction and start to move. This was demonstrated for KG lattices in \[16, 40\]. Extending this work it was shown that as one fundamental DB, say the site-centred, loses stability the bond-centred DB will instead gain stability and also have an eigenmode associated with this that can act as a depinning mode \[15, 48\]. Moreover, the two DBs do not change stability at exactly the same point and there is a small region where they both are either stable or unstable. In this region it is possible to show the existence of an intermediate DB solution that is centred neither on a site nor exactly inbetween sites. See Fig. 3 in paper II or Fig. 2 in paper V for examples in DNLS models.

The intermediate solution appears from a bifurcation when the site-centred DB loses stability and disappears in a bifurcation with the bond-centred DB when it gains stability, or vice versa. The intermediate solution will thus connect the two fundamental solutions in parameter space \[15, 48\]. Since the eigenmodes involved in the change of stability promote a change of form, and also a change of form of one fundamental mode into another, again exemplified in Fig. 3 in paper I, we are lead to the heuristic view of mobility of the highly localized modes as a transformation of one stationary mode into the other via the intermediate solution. In this context the concept of the PN-barrier makes great sense, since in connection with the inversion of stability between the two fundamental modes the energy difference will vanish. In a Hamiltonian system, the solution with lowest energy will be stable (a proof for DNLS equations can be found in \[201\]), and thus the inversion of stability involving the lowest energy mode will always be connected to a vanishing energy difference. This does not mean that the PN-barrier will be zero. The energy of the intermediate solution must also be taken into account when the PN potential is considered for stationary solutions. This means that if the travelling excitation is not an exact solution it will eventually get pinned as some energy is radiated away. This radiation can be very small and the highly localized excitation can essentially propagate indefinitely, as has been observed in several numerical simulations \[15, 16, 48\] (see also paper I). It has also been shown numerically, that exact localized travelling solutions without oscillations in the tail can exist at so-called transparent points \[45\]. This will occur when the energy difference of site-centred and bond-centred solutions vanish exactly at the same parameter values as when the stability is interchanged between them.\[25\] The velocity of these exact travelling solutions must always be finite, since at low velocity there will be resonances with linear modes. This is in contrast to the exact solutions of the integrable models.

The DNLS models which exhibit a reduced PN-barrier are, e.g., used as models for arrays of coupled optical waveguides, and the existence of narrow travelling...
excitations are therefore very interesting from an application point of view. Since mobility can be induced by simple perturbations the prospects for using these systems as switches are promising. Experimentally, a kick similar to a depinning mode is, e.g., easily achieved by applying a phase gradient to the stationary solution.

### 1.2.7 Compactness

The localized discrete solutions we have considered this far are generally exponentially localized in the lattice. For lattices on the form of Eq. (1.21), with nearest-neighbour coupling, a tail analysis at small amplitudes would lead us to consider the linear equation (1.22). For a stationary tail, the only spatially decaying solution of the resulting recurrence relation is exponentially decaying. With the discovery of compactons in continuum systems (Sec. 1.1.3), the search for compact DBs, i.e., excitations without of a decaying tail, were inspired also in lattices. In discrete systems the analogue of nonlinear dispersion is a nonlinear coupling, and it was pointed out [112] that a purely nonlinear coupling could lead to compactification of an intrinsic localized mode. The compact solutions in [112] were later shown not to be strictly compact, but to have a superexponential decay [75]. Generally, in models on the form of Eq. (1.21) there can be no exact compact DBs, but the superexponential decay of a localized mode occurs under general circumstances for a purely nonlinear polynomial coupling $W'$ [57, 69]. However, exact compact DBs are possible if the nonlinear couplings are of a more general form than in the model (1.21). Examples of such models, constructed from a reversed engineering approach, can be found in [111] (see also [110]). The key is to have a coupling that can vanish for a particular amplitude when one of the nearest neighbours has zero amplitude. This will effectively lead to a decoupling of the lattice between these sites and allow for a compact localized excitation.

The agreement between the superexponentially decaying DBs in models with a purely nonlinear coupling and their compacton counterparts in the corresponding continuum models with nonlinear dispersion can be very good [58]. This cannot be expected for the exact compact DBs. If the model has a linear coupling, that can be balanced by a nonlinear coupling so the total coupling becomes zero [57] the corresponding continuum equation would have a linear dispersion term. As remarked in section 1.1.3 this will rule out any compactons with a zero background. Hence, in some cases the property that allows for compact solutions in the discrete equation will prevent it in the corresponding continuum equation.

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33 Some details on how this occurs can be found in papers [111] and [110].
In this thesis we investigate the properties of some nonlinear Schrödinger equations, both spatially discrete and continuous, called so because of their resemblance to the wave equation of quantum mechanics. In the previous chapter we saw how such equations can arise as the limiting form of general dynamical equations. The purpose of this chapter is to demonstrate how these equations also arise in different physical contexts as models in their own right.

### 2.1 Dielectric waveguides

A basic feature of the Maxwell equations for the electromagnetic field is the existence of travelling waves which represent a transport of energy. Limiting our discussion to nonconducting media in the absence of sources the equations (in SI-units) take the form

\[
\begin{align*}
\nabla \cdot D &= 0, \\
\n\nabla \times E + \frac{\partial B}{\partial t} &= 0, \\
\n\nabla \cdot B &= 0, \\
\n\n\nabla \times H - \frac{\partial D}{\partial t} &= 0.
\end{align*}
\]

The displacement field and the electric field are related by \( D = \varepsilon E \), where \( \varepsilon \) is the permittivity or dielectric function. The magnetic flux density and the magnetic field satisfy \( B = \mu H \), where \( \mu \) is the permeability. For electromagnetic waves in a material we consider the charge polarization, or induced dipole moment per volume element, \( P \). For a dielectric material it holds that \( D = \varepsilon E = \varepsilon_0 E + P \), i.e., the charge polarization describes the difference from vacuum due to the presence

\[1\] See, e.g., [41, 97] for general references on electromagnetic theory.
of the material. Under these assumptions Eqs. (2.1) can be combined to yield the wave equation

$$\left( \nabla^2 - \mu \epsilon_0 \frac{\partial^2}{\partial t^2} \right) E(r, t) = \mu \frac{\partial^2}{\partial t^2} P(r, t). \quad (2.2)$$

This equation will be the basis of our analysis of nonlinear optical phenomena in dielectric materials. We will resort to approximations, here by taking a perturbative approach and treating the nonlinear effects as small deviations from the linear theory. For dielectric waveguides a perturbation theory has been developed under the name coupled-mode theory (section 2.1.1). The predictions made using this theory for coupled (nonlinear) optical waveguides are, as we shall see, well supported by experiments.

For a uniform linear medium, with $P = (\epsilon - \epsilon_0)E$ and $\epsilon$ a constant, we consider as a possible solution of Eq. (2.2) a wave travelling in the $z$ direction on the form $E(r, t) = E(x, y)e^{i(\beta z - \omega t)}$, which is to satisfy the Helmholtz equation

$$\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) E(x, y) + (\mu \epsilon \omega^2 - \beta^2) E(x, y) = 0. \quad (2.3)$$

The corresponding magnetic field $H$ can be obtained from Eqs. (2.1).

In an unbounded region we may take $E(x, y) = \text{constant}$ to get a plane wave with the dispersion relation $\beta = \sqrt{\mu \epsilon \omega}$ between the wave number $\beta \equiv k_z$ and the frequency $\omega$. The phase velocity of the wave is

$$v = \frac{\omega}{\beta} = \frac{1}{\sqrt{\mu \epsilon}} \frac{c}{n}, \quad n = \sqrt{\frac{\mu \epsilon}{\mu_0 \epsilon_0}}, \quad (2.4)$$

where $c = (\mu_0 \epsilon_0)^{-1/2}$ is the velocity of light in vacuum and $n$ is the index of refraction.

Considering instead a bounded region we can, without explicitly solving the Helmholtz equation (2.3), still draw some important conclusions as to the behaviour of the general solutions, primarily by considering the sign of the quantity $\mu \epsilon \omega^2 - \beta^2$. If it is positive the solutions will be oscillating in nature and if it is negative they will have an exponential character, although the exact behaviour depends on boundary conditions. The key idea of a hollow dielectric waveguide is to confine the electromagnetic wave in the directions transverse to the direction of propagation, i.e., to guide the wave. By suitably choosing the physically tunable parameters, the frequency $\omega$ and the material parameters $\mu$ and $\epsilon$, a wave can be guided in the $z$ direction if a region in the transverse direction of higher index of refraction is bounded by a region of lower index of refraction. Such a wave will mainly be restricted to the interior region with an evanescent, exponentially decaying, tail in the exterior region. At the interface we must require that the tangential components of the $E$ and $H$ fields are continuous. These boundary conditions will impose restrictions on the confined solutions, leading to a quantization of the transverse components of the wave vector $k$ and subsequently allow only for a discrete (infinite) set of confined solutions $E^{(\nu)}$ to (2.3), called the confined or guiding modes of the waveguide. Since the total wave number $k = |k|$ is related to the frequency $\omega$ through the dispersion relation $k = \sqrt{\mu \epsilon \omega}$, there will also be
2.1 Dielectric waveguides

a corresponding set of propagation constants $\beta_\nu$ (the $z$-component of the wave vector). Depending on the frequency, the matching $\beta_\nu$ will either be real, meaning that the confined mode will be a propagating mode, or purely imaginary, meaning that the fields will decay in the direction of propagation. Generally, the frequency is chosen so that only one or a few modes are propagating. This is referred to as single-mode and multi-mode propagation, respectively. Apart from the confined modes there is also a continuum of solutions that are oscillating in both the interior and the exterior region. These are referred to as radiation modes and represent a transfer of energy away from the interior region of the waveguide.

For hollow metallic waveguides of uniform cross section there are some simplifying properties for the waveguide modes. It is, for example, possible to categorize the modes in transverse electric (TE) and transverse magnetic (TM) modes, meaning that they have, respectively, no electric or magnetic field component in the propagating direction. For dielectric waveguides this is in general not true since the longitudinal electric and magnetic field components will couple to each other. However, the distinction between TE and TM modes holds for a slab dielectric waveguide and also in general for any azimuthally symmetric mode, like the lowest modes of a circular dielectric waveguide. This is also approximately true for the lowest modes of a rectangular dielectric waveguide, where the field in one of the transverse directions of polarization dominate over the longitudinal direction. Thus, for simplicity, we keep the distinction between TE and TM modes in the following presentation. This has no impact on the formulation of the coupled-mode theory. A further simplifying property is the orthogonality of the modes, in the sense that

$$\int \int E^{(\nu)} \cdot E^{(\lambda)} \, dx \, dy = \int \int H^{(\nu)} \cdot H^{(\lambda)} \, dx \, dy = 0, \quad \nu \neq \lambda. \quad (2.5)$$

A convenient way to deal with the normalization of the waveguide modes comes in relation to the power carried by the electromagnetic field. This is described by the Poynting vector $S = \frac{1}{2} (E \times H^*)$, which is the time-averaged flux of energy. To evaluate the total power flow $P$ along the waveguide we integrate the $z$-component of $S$ over a cross section of the waveguide. From the orthogonality properties, Eq. (2.5), of the modes it follows that the power carried by a given mode is

$$P = \frac{1}{2} \int \int (E^{(\nu)} \times H^{(\nu)}) \cdot \hat{z} \, dx \, dy. \quad (2.6)$$

Using that the transverse field components are related by

$$H^{(\nu)}_t = \frac{1}{Z_\nu} \hat{z} \times E^{(\nu)}_t, \quad Z_\nu = \begin{cases} \frac{\mu_0 \omega}{\beta_\nu} & \text{(TE)} \\ \frac{\beta_\nu}{\epsilon_0 \omega} & \text{(TM)} \end{cases} \quad (2.7)$$

where $Z$ is the wave impedance, the expression for the power can be evaluated to

$$P = \frac{1}{2Z_\nu} \int \int |E^{(\nu)}_t|^2 \, dx \, dy. \quad (2.8)$$

See [138] for an approximate solution of the rectangular waveguide. Modes with both electric and magnetic components in the propagating direction are called hybrid modes.
If the mode is normalized so that \( P = P_0 \) [W], a field \( \mathbf{E} = \Psi \mathbf{E}^{(\nu)} e^{i(\beta_\nu z - \omega t)} \), where \( \Psi \) is a complex amplitude, will correspond to a power flow of \( |\Psi|^2 P_0 \) [W].

### 2.1.1 Coupled-mode theory

To develop a perturbation theory for electromagnetic waves we will consider the charge polarization \( \mathbf{P} \) of the guiding medium. Assume that we apply a perturbation to a system modelled by Eq. (2.2) and that this perturbation can be described by a change \( \mathbf{P}' \) in the charge polarization \( \mathbf{P}_0 \) of the unperturbed system, \( \mathbf{P} = \mathbf{P}_0 + \mathbf{P}' \). If \( \mathbf{D} = \epsilon \mathbf{E} = \epsilon_0 \mathbf{E} + \mathbf{P}_0 \), so that \( \epsilon \) is the dielectric constant of the unperturbed system, the equation for the perturbed system takes the form

\[
\left( \nabla^2 - \mu \epsilon \frac{\partial^2}{\partial t^2} \right) \mathbf{E}(r, t) = \mu \frac{\partial^2}{\partial t^2} \mathbf{P}'(r, t). \tag{2.9}
\]

The type of perturbations that can be incorporated in \( \mathbf{P}' \) are, e.g., effects of changing material parameters and spatial deformations to the medium that guides the electromagnetic wave.

When this perturbative approach is applied to waveguides it goes under the name coupled-mode theory [202, 203]. The key idea is to expand the total field in the perturbed waveguide as a superposition of the orthonormal modes of the unperturbed waveguide. Essentially, we assume that the perturbation can be absorbed in the expansion coefficients, or mode amplitudes. In this treatment we ignore the possibility of coupling to the continuum of radiation modes, meaning that no power is leaked from the waveguide, and we assume only propagation in the positive \( z \) direction. Finally, we will at this instant assume that the modes are real, which, e.g., is true if they have a preferred direction of polarization. Thus,

\[
\mathbf{E}(r, t) = \frac{1}{2} \sum \Psi_\nu(z) \mathbf{E}^{(\nu)}(x, y) e^{i(\beta_\nu z - \omega t)} + c.c., \tag{2.10}
\]

where \( \mathbf{E}^{(\nu)} \) are the confined modes satisfying Eq. (2.3) with corresponding propagation constants \( \beta_\nu \).

Substitution of Eq. (2.10) in Eq. (2.9) leads to

\[
\frac{1}{2} \sum \Psi_\nu \left[ \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \mathbf{E}^{(\nu)} + (\mu \epsilon \omega^2 - \beta_\nu^2) \mathbf{E}^{(\nu)} \right]
+ \left[ \frac{\partial^2 \Psi_\nu}{\partial z^2} + 2i\beta_\nu \frac{\partial \Psi_\nu}{\partial z} \right] \mathbf{E}^{(\nu)} e^{i(\beta_\nu z - \omega t)} + c.c.
= \mu \frac{\partial^2}{\partial t^2} \mathbf{P}'(r, t), \tag{2.11}
\]

where the expression in the first bracket vanishes since \( \mathbf{E}^{(\nu)} \) is a solution of the unperturbed system (2.3). If further a slow variation of the mode amplitudes is

\[\text{If there is a } z \text{ dependence of the perturbation to the system, we would in principle also need to consider backward propagating fields due to scattering.}\]
Eq. (2.11) simplifies to

\[ \sum_{\nu} i \beta_{\nu} \frac{\partial \Psi_{\nu}}{\partial z} e^{i(\beta_{\nu} z - \omega t)} + c.c. = \mu \frac{\partial^2}{\partial t^2} P'(r, t). \]  

Multiplying with \( E^{(\nu)} \) and integrating over the transverse directions we arrive at, using Eq. (2.5), an equation for the evolution of the mode amplitudes

\[ i \frac{\partial \Psi_{\nu}}{\partial z} e^{i(\beta_{\nu} z - \omega t)} \iint |E^{(\nu)}|^2 \, dx \, dy + c.c. = \frac{\mu}{\beta_{\nu}} \frac{\partial^2}{\partial t^2} \iint E^{(\nu)} \cdot P'(r, t) \, dx \, dy. \]  

The normalization integral over the mode can in the case of TE modes be directly evaluated from Eq. (2.8), but for TM modes we also need to consider the longitudinal component of the electric field. Using the orthogonality properties, Eq. (2.5), it is possible to work out this contribution. In summary, the result is

\[ i \frac{\partial \Psi_{\nu}}{\partial z} e^{i(\beta_{\nu} z - \omega t)} + c.c. = \begin{cases} \frac{1}{2 \omega P_0} \frac{\partial^2}{\partial t^2} \iint E^{(\nu)} \cdot P'(r, t) \, dx \, dy, & \text{(TE)} \\ \frac{1}{2 \omega P_0} \frac{\mu \omega^2}{2 \beta^2_{\nu} - \mu \omega^2} \frac{\partial^2}{\partial t^2} \iint E^{(\nu)} \cdot P'(r, t) \, dx \, dy, & \text{(TM)} \end{cases} \]  

where \( P_0 \) is the normalized power. In Sec. 2.1.3 we will apply these formulas for the coupling of modes between guides in an array, but first we need to consider the effects of nonlinear materials.

### 2.1.2 Nonlinear optical effects

At optical and infrared frequencies the responses of a material to an external electric field are mainly electronic in nature. It can be understood as a relative displacement of the electronic density around the atoms and molecules that constitute the material due to the force from the applied field. The result is an induced dipole moment, which from a macroscopic viewpoint is described by the charge polarization \( P \). Even if the external field is a light beam it is often sufficient to treat only effects of the electric part of the electromagnetic wave, since the force from the magnetic part has a much weaker influence on electrons.

---

4The Lorentz force on a particle moving in an electromagnetic field is \( \mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \).

For an optical field the magnitudes of the electric field and the magnetic flux density are related by \( |\mathbf{B}| = \frac{\mu_0}{\mu_0} |\mathbf{E}| \sim 10^{13} |\mathbf{E}| \). Further, the electrons are oscillating with the optical frequency \( f \sim 10^{15} \) Hz on an atomic length-scale \( a \sim 10^{-10} \) m. Hence we estimate \( |\mathbf{v}| \sim fa \sim 10^7 \) m/s and the contribution to the force from the magnetic part of the optical field is about three orders of magnitude less than the electric part.
The restoring force on the electrons due to the positive nucleus is very strong and corresponds to an electric field of the order of $10^{10}$–$10^{11}$ V/m. Hence, at low field strengths compared to the internal field the displacements of the electrons are, to a very good approximation, proportional to the applied electric field, i.e., $P = \epsilon_0 \chi E$, where $\chi$ is the electric susceptibility. It was only with the development of the laser, which is capable of producing optical electric fields of $10^8$–$10^9$ V/m, that a significant deviation from the linear behaviour could be detected. This was first done in 1961, when P. Franken and co-workers observed second harmonic generation (frequency doubling) in a quartz crystal. However, this was not the first nonlinear optical effect observed. Already at the end of the 19th century J. Kerr conducted an experiment that showed a nonlinear interaction between electromagnetic fields and matter. He observed that a static electric field in a piece of glass induced birefringence. This means that the phase velocity of an electromagnetic wave propagating in the material depends on the polarization of the wave, one consequence being that linearly polarized light can emerge elliptically polarized after passing through the material. This is a general property of anisotropic materials, but in this case the anisotropy was induced by the applied field. Lower field strengths are sufficient for such effects, involving static or near-static electric fields, since they are mainly related to a reorientation of the prolonged molecules in the material and not to a direct response of the electrons. Therefore longer response times are also to be expected.

In principle, when a strong optical electric field is applied, the redistribution of charge would itself affect the internal field of the atom or molecule, due to a change in effective screening. Hence, the restoring force will no longer be proportional to the electronic displacement and the response will be nonlinear. From the macroscopic viewpoint, this means that the induced charge polarization $P$ has a nonlinear dependence on the applied field $E$. In this limited account of nonlinear optical effects we will make a few simplifying assumptions as to not cloud our description with unnecessary formulas. The focus will be on phenomenological aspects and we refer, e.g., to [28] for a more complete treatment. If we assume that the responses to the applied field are instantaneous, which amounts to neglecting the contribution of molecular vibrations or the Raman effect, and if we also assume that the material is isotropic, a power series expansion of the polarization would be

$$P = \epsilon_0 \chi^{(1)} E + \epsilon_0 \chi^{(2)} EE + \epsilon_0 \chi^{(3)} EEE + \cdots,$$

where $EE$ is a tensor product. The susceptibilities $\chi^{(n)}$ are in general rank $(1, n)$.
tensors connecting the various components of the electric field with the charge polarization. Further, all even-order susceptibilities will vanish if the material has inversion symmetry, for which isotropy is a sufficient but not a necessary condition. Such materials, where the lowest-order nonlinear effect is governed by the third order susceptibility, are generally called Kerr materials and will be the focus of our further studies. Under the assumptions made we can in fact take a scalar approach to the fields, since in a non-birefringent material the direction of polarization of the electric field will be maintained. We take the applied field as a quasi-monochromatic optical field,

\[
E(r, t) = \frac{1}{2} \left[ E(r, t) e^{-i\omega t} + E^*(r, t) e^{i\omega t} \right] \hat{e},
\]

where \( E(r, t) \) is slowly varying in time, compared to the optical period \( 2\pi/\omega \), and \( \hat{e} \) is the polarization unit vector. Note that the field is real, since when considering nonlinear effects we can no longer use the convenient notational convention of complex fields built on the principle of superposition. Upon inserting Eq. \( 2.17 \) into Eq. \( 2.10 \) we have

\[
P = \varepsilon_0 \chi^{(1)} E + \frac{3\varepsilon_0 \chi^{(3)}}{4} |E|^2 E + \varepsilon_0 \chi^{(3)} \left( E^* e^{-3i\omega t} + E^* e^{3i\omega t} \right) \hat{e} + \mathcal{O}(E^5). \tag{2.18}
\]

The terms with a time-dependence proportional to \( 3\omega \) must satisfy a phase-matching condition and are in general negligible. Since \( D = \varepsilon E = \varepsilon_0 E + P \), it follows that the lowest-order nonlinear dielectric function for a Kerr material is

\[
\varepsilon = \varepsilon_0 + \varepsilon_0 \chi^{(1)} + \frac{3\varepsilon_0 \chi^{(3)}}{4} |E|^2. \tag{2.19}
\]

For a non-magnetic material we can write this in terms of the more familiar index of refraction, \( n^2 = \varepsilon/\varepsilon_0 \),

\[
n = n_0 + n_2 |E|^2, \tag{2.20}
\]

where \( n_0 = \sqrt{\varepsilon_0 (1 + \chi^{(1)})} \) and \( n_2 = 3\chi^{(3)}/8n_0 \) is called the Kerr index, or Kerr coefficient, of the material.

---

8In general, Eq. \( 2.10 \) should be a tensor relation written in Fourier space where \( \chi^{(n)} \) can be complex and depends on the frequencies of the applied field. If the frequencies are far from resonances (excitation energies) of the molecules, the susceptibilities are real quantities. This means that no energy transfer occurs in the matter-field interaction, and that energy only is exchanged between different states of the electromagnetic field. The process is non-resonant. With a definite direction of polarization, say \( \hat{x} \), of the applied field the scalar quantities \( \chi^{(1)} \) and \( \chi^{(3)} \) appearing in our simplified equations are the components \( \chi^{(1)}_{xx} \) and \( \chi^{(3)}_{xxx} \) of the general tensors.

9The direction of polarization is unchanged also in a birefringent material if it coincides with one of the principal dielectric axes of the crystal.

10On the microscopic level the incoming and outgoing photon quanta must, apart from the energy conservation \( 3\omega = \omega + \omega + \omega \), satisfy a momentum conservation \( \Delta k = k(3\omega) - 3k(\omega) = 0 \). The phase-mismatch \( \Delta k \) is a measure of the interference of the waves with different frequencies and \( \Delta k = 0 \) can only be satisfied if \( n(3\omega) = n(\omega) \), which we obtain from Eq. \( 2.14 \), on the form \( k(\omega)c = \omega n(\omega) \). Since the index of refraction generally increases with \( \omega \) this is not possible in a non-birefringent material.
It is also interesting to note that wave propagation in a nonlinear Kerr material will to first order be governed by a two-dimensional NLS equation. If we take the nonlinear part of Eq. (2.19) as a perturbation to the linear material the equation (2.9) will, with a field on the form

$$E(\mathbf{r},t) = \frac{1}{2} \Psi(\mathbf{r}) e^{i(\beta z - \omega t)} \hat{e} + c.c.,$$  

result in the equation

$$2i\beta \frac{\partial \Psi}{\partial z} + \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + 2\frac{\beta^2 n_2}{n_0} \Psi |\Psi|^2 = 0,$$  

where $\beta^2 = \mu \epsilon \omega^2$ and the envelope $\Psi$ is assumed to be slowly varying in $z$ compared to the wavelength of the field (cf. Eq. (2.12)). With the nonlinear induced change of the index of refraction, a beam governed by Eq. (2.22) can self-focus ($n_2 > 0$) by essentially creating its own waveguide \[12\]. However, in two spatial dimensions solitons in a Kerr material are unstable and will generally be subjected to a collapse phenomenon, where the power is focused into a very narrow region in finite time \[24, 167\]. Supressing the diffraction in one dimension, by confinement in a slab waveguide, Eq. (2.22) will reduce to the one dimensional NLS equation where stable propagation of solitons is possible. See \[114\] for a thorough account of the theory and experiments.

To come close to these ideal situations in experiments it is important to avoid absorption, manifested as an imaginary part of the index of refraction, due to energy exchange between the light beam and the material. This is best achieved when the photon energy used for experiments is far from resonances with any transition energies in the atoms or molecules making up the material. Apart from absorption, the resonances can also modify the nonlinear change of the index of refraction, making higher-order susceptibilities non-negligible or resulting in a saturation of the nonlinearity \[132\]. Thus, other nonlinear dependencies than in Eq. (2.22) are possible. Spatial solitons in pure Kerr media have been observed in silica glasses \[7\]. Unfortunately, the nonlinearity $n_2 \simeq 8 \times 10^{-23} \text{m}^2/\text{V}^2$ ($\hat{n}_2 \simeq 3 \times 10^{-16} \text{cm}^2/\text{W}$) is small, implying high intensities of a few TW/cm$^2$ for the formation of solitons \[4\]. The intensities are so high that laser pulses of duration no longer than a few femtoseconds must be used in order to prevent material damage. However, there are other glasses with stronger nonlinearity that as a consequence require lower intensities for solitons \[132\] \[14\]. More interesting materials are semiconductors, like AlGaAs, with lasers operating at photon energies below one-half of the semiconducting bandgap energy, corresponding to a wavelength of $\lambda_{\text{gap}} = 0.75 \mu\text{m}$ \[105\]. One-photon absorption is low and two-photon absorption is in principle forbidden, so losses are low. Crystals several centimetres long and pure

\[11\] Here $n_2$ refers to the Kerr index defined by the relation $n = n_0 + n_2 |E|^2$. It is also common to use $n = n_0 + n_2 I$, where $I = (c \mu_0)^{-1} |E|^2$ is the intensity. Note also that the spatial extent of the soliton in the transverse directions is of the order $k_0^{-1} \simeq \sqrt{n_0/2\beta^2 n_2 \mu_0 I} \sim 10^{-4} \text{m}$.

\[12\] We should also note that for temporal solitons, i.e., pulses localized in time, that are propagating in an optical fibre, weaker nonlinearities are sufficient. This is because the effect of dispersion in the fibre is weaker than the effect of diffraction in bulk media \[114\].
2.1 Dielectric waveguides

enough for low scattering losses are easily fabricated [132]. Since the nonlinear index of refraction is \( n_2 \approx 5 \times 10^{-20} \text{ m}^2/\text{V}^2 \) \( (\hat{n}_2 \approx 2 \times 10^{-13} \text{ cm}^2/\text{W}) \) for wavelengths of about \( \lambda \approx 1.55 \mu\text{m} \), typical soliton intensities are in the GW/cm\(^2\) regime [6]. Also, a negative Kerr index of \( n_2 \approx -3 \times 10^{-19} \text{ m}^2/\text{V}^2 \) \( (\hat{n}_2 \approx -10^{-12} \text{ cm}^2/\text{W}) \) can be achieved for AlGaAs at wavelengths corresponding to photon energies just below the bandgap. But as the bandgap is approached losses from absorption greatly increase [126]. Materials with negative Kerr index are called de-focusing and do in general support so-called dark solitons, i.e., solutions with a constant non-zero background intensity and a localized dip where the intensity goes to zero (see further Sec. 3.1.2) [114]. Solitons are also of interest in non-Kerr materials where other processes than charge polarization is the source of the nonlinearity. In photorefractive materials, e.g., strontium barium niobate, lithium niobate or barium titanate, an external field is used to change and activate a nonlinear change of the index of refraction for a probing beam by inducing charge carriers that locally screen the field of the beam [132]. The beam propagation can be accurately modelled by NLS equations with saturating nonlinearity [44]. With such a nonlinearity two-dimensional solitons can be stable, since the saturation will arrest the collapse otherwise present in Kerr media with a cubic nonlinearity.

2.1.3 Coupled waveguides

Placing two, or more, waveguides in close proximity the modes of the respective guides will couple to each other due to an evanescent field overlap, leading to a power exchange between the waveguides known as directional coupling [202]. This coupling can be described within the theory of Sec. 2.1.1. The idea is to study a single isolated waveguide and to consider the effect of neighbouring waveguides and nonlinear responses of the guiding medium as perturbations.

In Fig. 2.1 a schematic one-dimensional array of optical waveguides is depicted.

![Figure 2.1](image)

**Figure 2.1.** An array of optical waveguides in a nonlinear material. The profiles of the different indices of refraction across the array are also shown. The linear index of the array is \( n_c(x, y) \), the linear index of a single isolated waveguide is \( n_m(x, y) \) and the Kerr index is \( n_2(x, y) \).
Assuming that any nonlinearities are of Kerr type, the index of refraction of
the full array is \( n(r, t) = n_c(x, y) + n_2(x, y)|E(r, t)|^2 \), from which we can determine
the deviation from a single isolated linear waveguide with index of refraction \( n_m(x, y) \).
The total charge polarization of the array is \( P = D - \epsilon_0 E = (n^2 - 1)\epsilon_0 E \), while
the polarization of a single waveguide is \( P_m = (n_m^2 - 1)\epsilon_0 E \). Hence, the perturbing
polarization is
\[
P' = P - P_m = (n_c^2 - n_m^2)\epsilon_0 E + 2n_c n_2 \epsilon_0 |E|^2 E, \tag{2.23}
\]
where only terms to first order in the Kerr index \( n_2 \) are kept.

The geometry of the waveguides can be quite arbitrary, but we will still make
some restrictions. It is assumed that the fields are decaying sufficiently fast outside
the waveguides to motivate coupling only to nearest neighbours. The dimensions
of the waveguides and the frequency \( \omega \) of the guided field are chosen to permit
only single-mode propagation, which in the simplest configurations in general will
mean that the propagating mode is a TE mode. If the electric field has a preferred
direction of polarization \( \hat{e} \), the modes can be assumed to be real. With identical,
equally spaced waveguides the total field in the \( m \)th waveguide is
\[
E_m = \frac{1}{2} (\psi_{m-1}\epsilon_{m-1} + \psi_m\epsilon_m + \psi_{m+1}\epsilon_{m+1}) e^{i(\beta z - \omega t)} \hat{e} + c.c., \tag{2.24}
\]
with \( \epsilon_{m\pm 1}(r) = \epsilon_m(r \mp d) \), \( d \) being a translation vector between adjacent waveguides.
The generalization to two spatial dimensions is straightforward, the main
difference for a square lattice being that there are now four nearest neighbours to
each waveguide and that the subscript \( m \) is replaced by two indices \( m, n \) enumerating the waveguides in the different directions. Sticking to the nearest-neighbour approximation, the quadratic term of the nonlinear index of refraction in Eq. (2.20)
is given by (compare Eqs. (2.17) and (2.24))
\[
|E_m|^2 \approx |\psi_{m-1}|^2 \epsilon_{m-1}^2 + |\psi_m|^2 \epsilon_m^2 + |\psi_{m+1}|^2 \epsilon_{m+1}^2
+ (\psi_{m-1}\psi_m^* + \psi_{m-1}^*\psi_m)\epsilon_{m-1}\epsilon_m
+ (\psi_m\psi_{m+1}^* + \psi_m^*\psi_{m+1})\epsilon_m\epsilon_{m+1}. \tag{2.25}
\]
Plugging the field expressions into Eq. (2.23) and the coupled-mode equation (2.16)
we arrive at, after equating terms in \( e^{i(\beta z - \omega t)} \) and its complex conjugate, the
equation
\[
\frac{i d\psi_m}{dz} = Q_1 \psi_m + Q_2 \Delta \psi_m + 2Q_3 \psi_m |\psi_m|^2 \\
+ 2Q_4 [2\psi_m \Delta(|\psi_m|^2) + \psi_m^2 \Delta(\psi_m^2)] \\
+ 2Q_5 [2|\psi_m|^2 \Delta \psi_m + \psi_m^2 \Delta \psi_m^* + \Delta(|\psi_m|^2)], \tag{2.26}
\]
for the evolution of the amplitudes of the electric field in the waveguides. The
discrete two-point difference operator in one dimension is
\[
\Delta \psi_m = \psi_{m-1} + \psi_{m+1}, \tag{2.27}
\]
and Eq. (2.26) is straightforwardly generalized to two dimensions by replacing $\Psi_m \mapsto \Psi_{m,n}$ and for a four-fold symmetry using the four-point difference operator

$$\Delta \Psi_{m,n} = \Psi_{m-1,n} + \Psi_{m+1,n} + \Psi_{m,n-1} + \Psi_{m,n+1}. \quad (2.28)$$

The coupling constants $Q_1$–$Q_5$ depend on the indices of refraction and the overlap of the waveguide modes,

$$Q_1 = -\frac{\omega \epsilon_0}{4P_0} \iint (n_c^2 - n_m^2) \varepsilon_m^2 \, dx \, dy$$

$$Q_2 = -\frac{\omega \epsilon_0}{4P_0} \iint (n_c^2 - n_m^2) \varepsilon_{m\pm1}^2 \, dx \, dy \quad (2.29a)$$

$$Q_3 = -\frac{\omega \epsilon_0}{4P_0} \iint n_c n_2 \varepsilon_m^4 \, dx \, dy \quad (2.29b)$$

$$Q_4 = -\frac{\omega \epsilon_0}{4P_0} \iint n_c n_2 \varepsilon_{m\pm1}^2 \varepsilon_m^2 \, dx \, dy \quad (2.29c)$$

$$Q_5 = -\frac{\omega \epsilon_0}{4P_0} \iint n_c n_2 \varepsilon_{m\pm1}^3 \varepsilon_m \, dx \, dy = -\frac{\omega \epsilon_0}{4P_0} \iint n_c n_2 \varepsilon_{m\pm1}^3 \varepsilon_m \, dx \, dy. \quad (2.29d)$$

Each constant can be identified with a particular contribution from the perturbing polarization. $Q_1$ arises from the overlap of the mode with the adjacent waveguides and will only modify the effective propagation constant of the mode. This term can easily be made to vanish by the substitution $\Psi_m \mapsto \Psi_m e^{-iQ_1 z}$. The $Q_2$ term arises due to the presence of a mode in the neighbouring waveguides and leads to a linear coupling. Note that $Q_2$ in general is negative. $Q_3$ represents a nonlinear interaction of the mode with itself and can be either self-focusing ($n_2 > 0$) or self-defocusing ($n_2 < 0$). The $Q_4$ and $Q_5$ terms come from the nonlinear interaction of one mode with the modes in adjacent waveguides. An explicit calculation of the coupling parameters for a one-dimensional array of slab waveguides with the nonlinear material present only inbetween the waveguides can be found in Appendix A.1. For a two-dimensional system, depending on the symmetry of the lattice, there is also the possibility of nonnegligible linear coupling to next-nearest neighbours. However, as shown in Appendix A.2 for a lattice of square waveguides with experimentally relevant sizes, the linear diagonal coupling can be estimated to be an order of magnitude smaller than the linear direct coupling. Note also that Eq. (2.26) is a more general form of the rotating-wave approximation for the general FPU lattice, Eq. (1.45), to which it reduces for $2Q_3 = Q_4 = Q_5$.

Eq. (2.26) is the fundamental equation mostly studied in this thesis. Although the derivation was first published with paper I, the equation was originally derived for an array of slab waveguides in the Masters Thesis of A. Eriksson [70]. We are especially interested in the effects of the nonlinear coupling terms, as studied in papers I–III and V. The relative strengths of the parameters naturally depend

\[13\] In paper I the coupling coefficients all have the opposite signs, due to a small error in the derivation. However, this does not affect the physical properties, since they all are related to the relative signs of the parameters. The signs may also be changed by either of the transformations $z \mapsto -z$ or $t \mapsto -t$ (or equivalently $\beta \mapsto -\beta$ or $\omega \mapsto -\omega$).
on the waveguide configurations and we will in the following sections review some results of coupled optical waveguides.

2.1.4 Linear array

If the array is constructed from a linear material \((n_2 = 0)\), or if it is operated at low powers such that the nonlinear terms are negligible, Eq. \((2.26)\) reduces to the linear equation

\[ i \frac{d \Psi_m}{dz} = Q_1 \Psi_m + Q_2 (\Psi_{m-1} + \Psi_{m+1}). \]  

(2.30)

The general solution of this equation can be constructed by noting its connection to a recurrence relation for Bessel functions of the first kind. With all power initially launched in a single waveguide, \(\Psi_0(0) = 1\) and \(\Psi_{m \neq 0}(0) = 0\), the solution is given by \(203\)

\[ \Psi_m(z) = (-i)^m J_m(2Q_2 z) e^{-iQ_1 z}. \]  

(2.31)

Solutions with arbitrary initial conditions can then be obtained from this Green’s function by superposition. Similarly, the Green’s function for a two-dimensional array is obtained by a symmetric decomposition of the linear equation in two parts, one for each of the directions. Using the same recurrence relation for Bessel functions the result is

\[ \Psi_{m,n}(z) = (-i)^{m+n} J_{m+n}(4Q_2 z) e^{-iQ_1 z}. \]  

(2.32)

As seen for a one-dimensional array in figure \(2.2a\), the initially localized power spreads across the array by discrete diffraction, as we would expect in a linear system. The first experimental verification of waveguide directional couplers, demonstrating this behaviour, was made in 1973 \(189\). Due to the discrete nature of the array, the diffractive properties can be altered and the spreading of the initially localized pulse can be arrested. Inserting the plane wave \(\Psi_m(z) = A e^{i(km - \beta z)}\) into Eq. \(2.30\) we obtain the diffraction (or dispersion) relation \(\beta = Q_1 + 2Q_2 \cos k\), and define the diffraction coefficient \(D = \partial^2 \beta / \partial k^2 = -2Q_2 \cos k\). A striking feature of the discrete array of waveguides, as opposed to a homogenous medium, is the periodicity of \(D\). It follows, with \(Q_2 < 0\), that \(D > 0\) for \(0 \leq k < \pi/2\) and \(3\pi/2 < k < 2\pi\), as in homogenous media, but for \(\pi/2 < k < 3\pi/2\) the diffraction coefficient is negative and the diffraction is anomalous. These properties can be utilized by applying a phase gradient \((e^{i\beta m})\) to the initial solution. Experimentally this is achieved by launching the pulse at an angle to the array, in which case it will propagate across the array \(161\). Moreover, at \(k = \pi/2\) and \(k = 3\pi/2\) we have \(D = 0\) and there is no initial pulse broadening due to diffraction as depicted in figure \(2.2b\). However, as the pulse propagates the coherence of the complex phase is lost, i.e. the phase gradient changes, leading to increasing diffraction and a subsequent spreading of the pulse.

A device with interesting applications, called a two-waveguide directional coupler, can be constructed if the number of waveguides is limited to two. From
2. Dielectric waveguides

\[ \text{Figure 2.2.} \, (a) \, \text{The discrete diffraction of an initially localised pulse } [\Psi_m(0) = e^{-m^2/2}] \text{ in a linear array of waveguides.} \, (b) \, \text{Due to anomalous diffraction the pulse broadening can be initially halted by a phase gradient } [\Psi_m(0) = e^{-m^2/2}e^{i\pi m/2}]. \, Q_1 = 0 \text{ and } Q_2 = -1 \text{ was used for the calculations.} \]

Eq. (2.30) the solution when all power is initially launched into one waveguides is

\[
\begin{align*}
\Psi_0(z) &= \cos(Q_2z)e^{-iQ_1z}, \\
\Psi_1(z) &= -i\sin(Q_2z)e^{-iQ_1z},
\end{align*}
\]

and we see that the power will periodically oscillate between the two waveguides. Depending on the length of the device, the power can be arbitrarily divided between the two channels. The device can be used for power division, modulation and multiplexing/demultiplexing [203]. If the modes of the two waveguides have different propagation constants, leading to a phase mismatch between the modes, a complete power transfer will not occur. This can be engineered by using non-identical waveguides or with an external field applied over the coupler. The maximum fraction of power transferred is given by

\[
4Q_2^2 [4Q_2^2 + (\Delta \beta)^2]^{-1},
\]

where \(\Delta \beta\) is the phase mismatch. Using this property a directional coupler switch has been demonstrated [38].

2.1.5 Nonlinear array

Incorporating also nonlinear effects for the array of waveguides the transmission characteristics will drastically change, at least for high powers when the nonlinear effects are well pronounced. The lowest-order phenomenological model for a one-dimensional nonlinear array with a Kerr nonlinearity is the cubic DNLS
\( i \frac{d \Psi_m}{dz} = Q_1 \Psi_m + Q_2(\Psi_{m-1} + \Psi_{m+1}) + 2Q_3|\Psi_m|^2. \)  

(2.34)

The localized solutions of this equation have been shown to give a very good agreement with experiments. The first direct observation of discrete spatial optical solitons was made in 1998 [68]. When the Kerr index of the nonlinear material is negative \((n_2 < 0)\), so that \(Q_2 / Q_3 < 0\), another type of solution is allowed, the dark soliton kind [110, 186]. These have also been observed for an array constructed from a material with a positive Kerr index [137, 150]. The self-defocusing effect needed for a dark soliton to form was obtained by effectively changing the sign of the coupling \(Q_2\) by operating in the anomalous diffraction regime of the array.

From an application point of view, the possibility of beam steering across waveguide arrays is interesting as it could be used for multiport switching. Propagation across the array is accomplished by launching a pulse with a phase gradient in the array, see [5] for an overview of dynamics of discrete solitons. Experimentally, the steering of discrete solitons [151] as well as their interaction [144] has been demonstrated. A problem, however, is that the discrete soliton will lose some energy to radiation as it is not an exact travelling solution. For wide excitations, extended over several waveguides, the discrete soliton can traverse across many waveguides since in the continuum limit there is the exact soliton solution of the NLS equation, Eq. (1.14) \((\gamma = 0)\), but for switching purposes it is preferable with narrow excitations to unambiguously choose the output channel of the array. The highly localized excitations will though only move a few lattice site due the presence of the Peierls-Nabarro barrier of Eq. (2.34). As discussed in Sec. 1.2.6, with other forms of the nonlinearity it has been suggested that the PN barrier can be reduced, leading to a better mobility. A different approach, instead relying on the property of pinning, is to displace a highly localized DB a few waveguides by collision with an extended low-intensity transversely propagating beam [21].

In many cases, the self-interacting nonlinearity \((Q_3)\) is much stronger than the nonlinear coupling \((Q_4 \text{ and } Q_5)\), and the latter are therefore ignored as a first approximation. This seems to be well motivated by the correspondence between the solutions of Eq. (2.34) and the experimentally studied structures [68, 137, 143, 144, 150, 151]. In these setups both the waveguides and the medium surrounding them are constructed of nonlinear materials. If instead linear waveguides are assumed, embedded in a nonlinear medium, the effects of the inter-site nonlinearities will be strengthened compared to the on-site nonlinearity. An explicit example where these effects are not negligible is given in Appendix A together with estimates of relevant parameters in an experimental setup. Although there is yet no experimental confirmation, the inclusion of the nonlinear coupling in the one-dimensional model leads to a reduced PN barrier and the possibility of highly localized travelling excitations (paper I). See also paper V for an investigation of a two-dimensional array, where mobility is not achieved. A device with two waveguides and nonlinear coupling was studied already in 1982 by S.M. Jensen [99], who showed that self-trapping can occur also in such small systems provided the input power is large enough. The nonlinear transmission characteristics of this device.
can also serve as an optical logic gate.

Similar effects as discussed here for dielectric waveguides have also to some extent been observed for other systems of nonlinear waveguides, e.g., in bundles of optic fibres [160]. A recent interesting development is also the use of nonlinear photorefractive crystals, where an extraordinarily polarized probing beam can propagate in a periodic structure that is optically induced by interfering ordinarily polarized plane waves. With these optically induced waveguides the properties of the system are easily tuned. Observation of nonlinear localization has been made in both one- and two-dimensional systems [51 52 53 163].

2.2 Coupled Bose-Einstein condensates

The transition of an ultracold collection of bosonic atoms, with temperature of a few $\mu$K, from a gaseous state to a collective state, signified by a macroscopic population of the lowest-energy quantum mechanical ground state, was originally predicted by A. Einstein in 1925 after initial ideas by S.N. Bose [27 66 67]. The formation of this Bose-Einstein condensate (BEC) is possible when the thermal de Broglie wavelength of the atoms becomes larger than the mean interparticle distance. This means that the wave functions of the individual atoms are considerably overlapped and interlaced, practically indistinguishable from each other. As such they can start to act as a whole, as a single collective coherent matter wave or condensate. The experimental realization of BECs was achieved in 1995 by confining a dilute gas of alkali atoms in a magnetic trap and using different techniques to cool the atoms below the critical temperature for condensation [10 56]. The number of atoms typically ranges from a few thousand to several millions and the condensate typically extends over a few hundred $\mu$m [53]. See also [162 165] for an introduction to the theory of Bose-Einstein condensation.

Using mean-field theory an equation describing the evolution of the collective wave function $\Phi(r, t)$ of the condensate can be derived from the many-body Hamiltonian describing the interaction of bosons [53 165]. The equation is known as the Gross-Pitaevskii equation,

$$i\hbar \frac{\partial \Phi(r, t)}{\partial t} = \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(r) + g|\Phi(r, t)|^2\right] \Phi(r, t). \tag{2.35}$$

The external potential $V_{ext}$ can for the magnetic trap be safely approximated with a harmonic potential $V_M(r) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$. Typical frequencies in the experimental setups are in the order of 10–1000 Hz [10 56]. The nonlinear term arises from an effective potential taking into account the atom-atom interaction, and the constant $g$ is given by

$$g = \frac{4\pi \hbar^2 a}{m}. \tag{2.36}$$

---

14 From statistical mechanics this is given by $\lambda_{dB} = \hbar/\sqrt{2\pi mk_B T}$, where $\hbar$ is Planck’s constant, $m$ the mass of the atoms, $k_B$ Boltzmann’s constant and $T$ the temperature [165].

15 $\Phi(r, t)$ is defined as the expectation value of the bosonic field operator in second quantization. This means that $|\Phi(r, t)|^2$ is the density of the condensate, which motivates the treatment of $\Phi(r, t)$ as a wave function.
The scattering length $a$ is related to the interaction of the atoms and is positive (negative) for an effective interatomic repulsion (attraction). Experimentally measured values for the alkali atoms are $a = 2.75$ nm for $^{23}$Na, $a = 5.77$ nm for $^{87}$Rb and $a = -1.45$ nm for $^7$Li (see [53] and references therein). The Gross-Pitaevskii equation (2.35) is an extension of the NLS equation (1.11) and supports solitons, that have been observed experimentally [29, 191].

Now, with an applied external optical standing wave, created from two laser beams propagating in opposite directions, a lattice can be created for the condensate. This was experimentally verified in [9]. In contrast to the case of optical waveguides, where a material is used to confine and guide a light wave, a laser is now used to confine and manipulate a matter wave. The optical potential is

$$V_{\text{opt}} = V_0 \sin^2(kx),$$  \hspace{1cm} (2.37)

where $k = 2\pi/\lambda$ and $\lambda$ is the wavelength of the laser, so the spacing of the lattice is $\lambda/2$. This potential will lead to a one-dimensional lattice with condensates occupying the sites of the lattice, but also lattices in two [90] and three [91] dimensions can be created with standing light waves in other directions. It is also possible to form 'superlattices' by using two standing waves of different wavelengths [158]. The energy barrier between adjacent sites, $V_0$, is determined by the intensity of the laser, and can be tuned from a regime where the condensates interact strongly to a regime where they for all practical purposes are isolated. Locally, at each site, the optical potential can be approximated with a harmonic potential

$$\frac{m}{2} \tilde{\omega}_x^2 (x - x_j)^2,$$

where $x_j = j\lambda/2$ is the position of the potential minimum and $\tilde{\omega}_x = \sqrt{2V_0k^2/m}$. In typical experiments $\tilde{\omega}_x \gg \omega_x$ and it is therefore convenient to write the external potential $V_{\text{ext}} = V_L + V_D$ as the sum of a confining lattice potential

$$V_L = V_0 \sin^2(kx) + \frac{m}{2} (\omega_y^2 y^2 + \omega_z^2 z^2)$$  \hspace{1cm} (2.38)

and a so-called driving field

$$V_D = \frac{m}{2} \omega_x^2 x^2.$$  \hspace{1cm} (2.39)

Physically the driving field can be interpreted as the effective force $F = -\partial V_D/\partial x$ acting on the center of mass of a condensate wave packet moving in the potential [187].

If the potential barrier is large enough[14] we may consider the lattice sites as occupied by individual condensates that are weakly interacting through tunnelling, i.e., we prescribe a wave function for each site of the lattice. The interesting dynamical quantities are the number of atoms $N_j(t)$ on each site and the relative phases $\theta_{j+1}(t) - \theta_j(t)$ of the condensates. In this tight-binding approximation we may write the condensate wave function as a sum over the weakly interacting wave functions at each well. With a separation of the temporal and spatial part the ansatz for the total wave function is

$$\Phi(\mathbf{r}, t) = \sum_j \Psi_j(t) \phi_j(\mathbf{r}),$$  \hspace{1cm} (2.40)

---

16Note that since the sign of the coefficient in front of the dispersion term ($\nabla^2$) is negative, $g < 0$ will now correspond to the focusing case.

17The BEC chemical potential $\mu$ should be much smaller than $V_0$. 
2.2 Coupled Bose-Einstein condensates

with \( \Psi_j(t) = \sqrt{N_j(t)} e^{-i\theta_j(t)} \). For the spatial profile of the wave function at each well, \( \phi_j(r) \), one can use the Wannier functions, which are real wave functions centred around the minima of the periodic potential and assumed to be sufficiently localized so that there is only a significant overlap with wave functions in the neighbouring potential wells \([187]\). They will be quasi-orthogonal, such that \( \int \phi_i^* \phi_j \, dr \approx 0 \) for \( i \neq j \). Inserting the ansatz \((2.40)\) into Eq. \((2.35)\), multiplying \( \phi_j \) and integrating over the spatial variables we arrive at the discrete equation

\[
\frac{i\hbar}{\Delta t} \frac{d\Psi_j}{d\tau} = \epsilon_j \Psi_j + \tilde{\epsilon} \Psi_j + K(\Psi_{j-1} + \Psi_{j+1}) + \chi_0 |\Psi_j|^2 \\
+ \chi_1 [2\Psi_j (|\Psi_{j-1}|^2 + |\Psi_{j+1}|^2) + \Psi_j^* (\Psi_{j-1}^* + \Psi_{j+1}^*)] \\
+ \chi_2 [2|\Psi_j|^2(\Psi_{j-1} + \Psi_{j+1}) + \Psi_j^* (\Psi_{j-1}^* + \Psi_{j+1}^*)] \\
+ \Psi_{j-1}|\Psi_{j-1}|^2 + \Psi_{j+1}|\Psi_{j+1}|^2.
\]

with constants

\[
\epsilon_j = \int V_D \phi_j^2 \, dr, \quad (2.42a) \\
\tilde{\epsilon} = \int \left[ \frac{\hbar^2}{2m} (\nabla \phi_j)^2 + V_L \phi_j^2 \right] \, dr, \quad (2.42b) \\
K = \int \left[ \frac{\hbar^2}{2m} \phi_j \cdot \nabla \phi_j \pm 1 + \phi_j V_{\text{ext}} \phi_j \pm 1 \right] \, dr, \quad (2.42c) \\
\chi_0 = g \int \phi_j^4 \, dr, \quad (2.42d) \\
\chi_1 = g \int \phi_j^2 \phi_{j \pm 1}^2 \, dr, \quad (2.42e) \\
\chi_2 = g \int \phi_j^3 \phi_{j \pm 1} \, dr = g \int \phi_j^3 \phi_{j \pm 1} \, dr. \quad (2.42f)
\]

This is on the form of Eq. \((2.20)\), apart from the site-dependent on-site energy \( \epsilon_j \). With a harmonic driving field \((2.39)\) we have \( \epsilon_j \propto j^2 \) and for a linear field \( \epsilon_j \propto j \). However, if the optical field \( V_{\text{opt}} \) is much stronger than the driving field \( V_D \) (\( \omega_r \gg \omega_x \)) the effects of this term will be small. Note also that to a first approximation (\( \chi_1 = \chi_2 = 0 \)) the dynamics is governed by a DNLS equation \([197]\). The nonlinear localization thus predicted has also been observed experimentally \([12]\). Numerical calculations for the spatial profile of the condensate wave functions support the approximations made in the derivation and also show that \( \chi_1 \) can be as small as two orders of magnitude less than \( \chi_2 \), and may therefore in many situations safely be neglected \([187]\). However, as \( N \chi_2/K \) can be of the order of 1, where \( N = \sum_j N_j \) is the total number of atoms in the condensate, the nonlinear coupling terms are important \([188]\).

In the tight-binding approximation it is implicitly assumed that the spatial part of the wave function \((2.40)\) does not depend on the number of atoms occupying a given site of the lattice. This is in general not true and motivates a generalization
of the ansatz to a nonlinear tight-binding approximation \[188\]

\[
\Phi(\mathbf{r}, t) = \sum_j \Psi_j(t) \phi_j(\mathbf{r}; N_j(t)).
\] (2.43)

This will introduce site- and time-dependent parameters in Eq. (2.41), since \(\phi_j\) implicitly depends on \(N_j\) and \(t\). However, the time-scale for the change of shape of the spatial wave function \(\phi_j\) is much faster than the time-scale connected to the dynamics of \(\Psi_j\), so the shape can be assumed to adjust adiabatically to the instantaneous number of atoms in each well. A further approximation that seems to work well is to expand \(\phi_j\) in the integrals (2.42) around the average number of atoms in each well and only keep the zeroth-order term, i.e., the parameters have a weak time-dependence. The most important consequence of the ansatz (2.43) is to modify the effective on-site nonlinearity. The term \(\chi_0 \Psi_j |\Psi_j|^2\) will be replaced by \(\chi_0^{(\alpha)} \Psi_j |\Psi_j|^\alpha\), where \(\alpha = 4/(2 + D)\) and \(D = 0, 1, 2, 3\) is the effective dimensionality of the condensates in the lattice. Roughly, \(D\) is the number of spatial directions in which the width of the condensate depends significantly on the number of atoms, which in principle is related to how the energy of the condensate compares to the confining potentials \[187, 188\].

The tight-binding approximation leading to the expansion in Eq. (2.41) is roughly equivalent to the expansion of the electric field in the modes of the individual waveguides in the context of coupled optical waveguides described in Sec. 2.1.3. In fact, we could have derived the discrete equation (2.26) in this fashion from Eq. (2.22) supplemented with a periodic potential representing the presence of the waveguides. Thus the Wannier function expansion is a general method for deriving discrete evolution equations from field equations in a strong periodic potential and could lead to similar equations also in other contexts \[8, 148\].

### 2.3 Continuum approximation

In a lattice, an excitation of large extension, or more precise, slowly varying in space compared to the distance between lattice sites, is likely to be quite insensitive to the discreteness. In such a situation it can be motivated to do a continuum approximation of the discrete system and replace the discrete field variable \(\Psi_m(t)\) with a continuous function \(\Psi(x, t)\) sampled at the lattice points. If we, without loss of generality, assume a unit lattice spacing, we formally write this as \(\Psi_m(t) = \Psi(x = m, t)\) for the amplitude at site \(m\). What we gain by this approach is a reduction of the system of coupled ordinary differential equations to a single partial differential equation. The discrete equations are said to be studied in the continuum limit. Under the assumption of slow variation, the amplitudes at different sites of the lattice can be related by a Taylor series expansion, which for nearest neighbours is

\[
\Psi_{m\pm 1}(t) = \Psi(x \pm 1, t) = \sum_{k=0}^{\infty} \frac{(\pm \partial_x)^k}{k!} \Psi(x, t) \equiv e^{\pm \partial_x} \Psi(x, t),
\] (2.44)
where $\partial_x = \partial / \partial x$ is the partial differential operator. Formally, this relation can be extended to relate any two sites of the lattice by $\Psi_{m+p}(t) = e^{i\partial_x} \Psi_m(t)$. For a two-dimensional square lattice the extension is trivial and we associate the continuous variables $x$ and $y$ with the discrete variables $m$ and $n$, respectively. The Taylor series relation is then generalized to $\Psi_{m+p,n+q}(t) = e^{i\partial_x} e^{i\partial_y} \Psi_{m,n}(t)$. A direct insertion of these relations into the discrete equations will produce an equation for the continuum limit, but there is a more conceptually appealing approach.

If the terms in Eq. (2.20) are slightly rearranged it can be written on the form

$$\frac{d\Psi_m}{dt} = (Q_1 + 2Q_2)\Psi_m + Q_2 \Delta_2 \Psi_m + (2Q_3 + 12Q_4 + 16Q_5) \Psi_m |\Psi_m|^2$$

$$+ 2Q_4 [2\Psi_m \Delta_2(|\Psi_m|^2) + \Psi_m^* \Delta_2(\Psi_m^2)]$$

$$+ 2Q_5 [2\Psi_m^2 \Delta_2 \Psi_m + \Psi_m^* \Delta_2 \Psi_m^* + \Delta_2 (\Psi_m |\Psi_m|^2)],$$

where $t$ is now used as the evolution variable (time) and $\Delta_2$ is the second-order difference operator or discrete Laplacian, $\Delta_2 \Psi_m = \Psi_{m-1} - \Psi_{m+1} - 2\Psi_m$. Taking the continuum limit of the equation may now be considered as replacing the discrete difference operators with the corresponding differential operators (see, e.g., [19, 110]). From Eq. (2.44) the operator $\Delta_2$ is in the continuum limit replaced by

$$\Delta_2 \mapsto e^{-\partial_x} + e^{\partial_x} - 2 = 4 \sinh^2(\partial_x/2).$$

Similarly in two spatial dimensions the discrete Laplacian $\Delta_2 \Psi_{m,n} = \Psi_{m-1,n} + \Psi_{m,n-1} + \Psi_{m+1,n} - 4\Psi_{m,n}$ is replaced with $\Delta_2 \mapsto 4 \sinh^2(\partial_x/2) + 4 \sinh^2(\partial_y/2)$. As yet we have made no approximation, and this substitution will keep all properties of the discrete system. One consequence is that the dispersion relation for the resulting partial differential equation is periodic. If the full spectral properties of $\Delta_2$ are retained we have made no real simplification. The differential operator in Eq. (2.46) is not very conveniently dealt with analytically and the periodicity of the dispersion relation also gives some numerical problems if the Fourier transform or, presumably, some other spectral method, is used to calculate derivatives. Hence, and here comes the approximation, a simpler expression for $\Delta_2$ will usually suffice and can be motivated for a slowly varying amplitude. The simplest approximation is just the second-order differential operator $\Delta_2 \mapsto \partial_x^2$. Under this substitution Eq. (2.45) results in the continuum equation

$$i \frac{\partial \Psi}{\partial t} = \alpha_1 \Psi + \alpha_2 \frac{\partial^2 \Psi}{\partial x^2} + \alpha_3 \Psi |\Psi|^2 + \alpha_4 \left(2\Psi \frac{\partial^2 |\Psi|^2}{\partial x^2} + \Psi^* \frac{\partial^2 |\Psi|^2}{\partial x^2} \right),$$

where the coefficients are related to the coupling constants of the discrete equation

---

18 In the Fourier domain spatial derivatives are related to the wave number by the correspondence $\partial_x \mapsto ik$. Inserting a plane wave $A e^{i(kx-\omega t)}$ will result in a dispersion relation $\omega \propto 4 \sin^2(k/2)$ in one dimension.

19 We have made use of the relation

$$2\Psi \frac{\partial^2 |\Psi|^2}{\partial x^2} + \Psi^* \frac{\partial^2 |\Psi|^2}{\partial x^2} = 2 |\Psi|^2 \frac{\partial^2 \Psi}{\partial x^2} + \Psi^2 \frac{\partial^2 \Psi}{\partial x^2} + \Psi \frac{\partial^2 |\Psi|^2}{\partial x^2}$$

to recognize that the nonlinear coupling terms have the same continuum limit.
The phonon spectrum of Eq. (2.47) will be unbounded, as is generally the case for partial differential equations. An improvement of the continuum approximation would be to keep the boundedness of the linear spectrum associated with the discrete equation. This is achieved by using a rational function approximation, or Padé approximant, of Eq. (2.46), which in lowest order is the pseudo-differential operator

$$\Delta_2 \mapsto \frac{\partial_x^2}{1 - \frac{1}{12} \partial_x^2},$$

(2.49)

Apart from an improved continuum approximation this operator is also the result when considering long-range dispersive interactions [84].

In paper II the continuum versions of Eq. (2.45) are considered, and it is shown that the pseudo-differential operator gives a better correspondence with the solutions of the discrete equation, than when using the second-order differential operator. Of interest is also that the nonlinear coupling terms give rise to nonlinear dispersive terms in the continuum equation, and with the right signs of the coefficients in Eq. (2.47) this will lead to the existence of exotic solitons (Sec. 1.1.3). These solutions will have discontinuous spatial derivatives, and as shown in paper II the exotic solitons of Eq. (2.47) will have infinite jumps in first derivative. Unphysical as this may seem, they are true solutions of the equation and discontinuities are not a problem when the underlying system actually is discrete. The discontinuities do, however, signal a breakdown of our approximations, since they implicitly contain a cut-off in wave number. The solutions can still be indicative of the behaviour of the system under study. Note also that, as indicated in [107], the inclusion of higher-order linear dispersive terms can have a smoothing effect on the solutions.

---

The rational function approximation $f(x) \sim n(x)/d(x)$ is done by considering the two polynomials $n(x) = n_0 + n_1 x + n_2 x^2 + \ldots$ and $d(x) = 1 + d_1 x + d_2 x^2 + \ldots$ and determining the unknown coefficients such that $f(x) d(x) - n(x) = O(x^m)$, i.e., when $f(x)$ is replaced with its Taylor expansion the expression should vanish to the desired order $m$. The expression Eq. (2.49) is good to order $O(\partial_x^m)$. 
Some properties of nonlinear Schrödinger equations

From the previous chapters it is clear that nonlinear Schrödinger models are used in a variety of different contexts, partly due to their generality in capturing the lowest-order effects of nonlinearity and dispersion/coupling. This chapter is devoted to the properties of these models and to the properties of their solutions.

3.1 Continuum equations

In Sec. 2.3 the equation

\[ i\Psi_t = \alpha_1\Psi + \alpha_2\Psi_{xx} + \alpha_3\Psi|\Psi|^2 + \alpha_4[2\Psi(|\Psi|^2)_{xx} + \Psi^*(\Psi^2)_{xx}], \]

(3.1)

where the subscripts now are used to denote partial derivatives, was derived as a continuum approximation of a discrete equation with nonlinear coupling. This is the equation studied in paper II and it will be used as the example in deriving properties of the continuum nonlinear Schrödinger equations. The starting point is noting that Eq. (3.1) can be derived from first principles, in the sense that it lends itself to a Lagrangian formulation. By this we mean that there is a Lagrangian

\[ L = \int L\,dx \]

(3.2)

and a Lagrangian density \( L \), which is a functional of the variables \( \Psi, \Psi_x, \Psi_t \) and their complex conjugates, such that the equation is a stationary point of the action integral

\[ S = \int L\,dt. \]

(3.3)
Thus the Euler-Lagrange equations resulting from the variation $\delta S = 0$ should produce Eq. (3.1). Since the field variables $\Psi = u + iv$ are complex the equation really represents two coupled real equations, ideally in the real and imaginary parts of the complex variables. The two coupled equations are then the result of the independent variation of $S$ with respect to the real variables $u$ and $v$. However, by the identities $u = (\Psi + \Psi^*)/2$ and $v = (\Psi - \Psi^*)/2i$ it follows, if $\Psi$ and $i\Psi^*$ are formally treated as independent variables\(^2\), that the variation with respect to the real variables can be written as

$$\frac{\delta S}{\delta u} = \frac{\delta S}{\delta \Psi} + \frac{\delta S}{\delta \Psi^*} = 0,\quad \frac{\delta S}{\delta v} = i \left( \frac{\delta S}{\delta \Psi} - \frac{\delta S}{\delta \Psi^*} \right) = 0. \tag{3.4}$$

From this set of equations it is obvious that we can instead take independent variations of $S$ with respect to $\Psi$ and $i\Psi^*$. The Euler-Lagrange equations are

$$\frac{\delta S}{\delta \Psi} = 0 \iff \frac{\partial L}{\partial \Psi} - \frac{d}{dx} \frac{\partial L}{\partial \Psi_x} - \frac{d}{dt} \frac{\partial L}{\partial \Psi_t} = 0, \tag{3.5a}$$

$$\frac{\delta S}{\delta \Psi^*} = 0 \iff \frac{\partial L}{\partial \Psi^*} - \frac{d}{dx} \frac{\partial L}{\partial \Psi^*_x} - \frac{d}{dt} \frac{\partial L}{\partial \Psi^*_t} = 0. \tag{3.5b}$$

It is now possible to find a Lagrangian density that from Eq. (3.5b) will give Eq. (3.1). If $L$ is real Eq. (3.5a) is just the complex conjugate of Eq. (3.5b), and we conclude that the Lagrangian density should be symmetric with respect to an interchange of the variables $\Psi$ and $i\Psi^*$. Thus, by inspection, the Lagrangian density is

$$L = \frac{i}{2} \Psi^* \Psi_t - \frac{\alpha_1}{2} |\Psi|^2 + \frac{\alpha_2}{2} |\Psi_x|^2 - \frac{\alpha_3}{4} |\Psi|^4 + \alpha_4 (\Psi^2 \Psi_x^2 + 2|\Psi|^2 |\Psi_x|^2) + c.c.. \tag{3.6}$$

### 3.1.1 Symmetries and conserved quantities

The real treat of the Lagrangian formulation is that it lets us relate some symmetry properties to quantities that are conserved under the dynamics governed by the equation. Apart from the fact that the conserved quantities give important information about the behaviour and properties of the system, they are also useful for controlling the accuracy and validity of numerical simulations. The formal relation between symmetries and conserved quantities for Lagrangian systems was first strictly formulated in a theorem by E. Noether \(^1\). The theorem concerns only continuous symmetries that can be expressed in terms of infinitesimal generators, and thus we introduce the small parameter $\epsilon$. Now, suppose that a transformation on the form

$$t \mapsto t + \epsilon T,$$

$$x \mapsto x + \epsilon X,$$

$$\Psi \mapsto \Psi + \epsilon \Upsilon,$$  

\(^1\)See the excellent book by H. Goldstein on classical mechanics \([87]\) for an account of Hamilton’s principle and the calculus of variations.

\(^2\)This is not a real problem since the relations between the two complex variables and the real variables define a canonical transformation (up to a scaling transformation). Some details can be found in the appendix of \([155]\).
3.1 Continuum equations

with \( T, X \) and \( \Upsilon \) functions of \( t, x, \Psi, \Psi_t \) and \( \Psi_x \), leaves the action integral \( S \) unchanged. Then the following continuity equation holds

\[
\frac{dI}{dt} + \frac{dJ}{dx} = 0, \tag{3.8}
\]

with

\[
I = \frac{\partial L}{\partial \Psi_t} (\Psi_t T + \Psi_x X - \Upsilon) + \frac{\partial L}{\partial \Psi_t^*} (\Psi_t^* T + \Psi_x^* X - \Upsilon^*) - LT, \tag{3.9}
\]

\[
J = \frac{\partial L}{\partial \Psi_x} (\Psi_t T + \Psi_x X - \Upsilon) + \frac{\partial L}{\partial \Psi_x^*} (\Psi_t^* T + \Psi_x^* X - \Upsilon^*) - LX. \tag{3.10}
\]

As pointed out already in Sec. 1.1.2 it follows by integration of Eq. (3.8) over \( x \) that \( I = \int I \, dx \) is a conserved quantity, or constant of motion, provided that the current density \( J \) approaches a constant value at infinity or if periodic boundary conditions are employed. The proof of the theorem, in the form of an explicit construction of the continuity equation from the transformation, can be found in [87], and a discussion in connection to nonlinear Schrödinger equations can be found in [167]. The transformation, Eq. (3.7), is quite general and the main conclusion of the theorem is that every continuous symmetry that can be represented on this form will yield a conserved quantity. However, nothing is said about other symmetries, like symmetry under inversion of time or some spatial coordinate. Further, the converse of the theorem is not true, i.e., there is not necessarily a symmetry related to every conserved quantity [87]. The most explicit examples are the integrable equations, like the cubic NLS equation, discussed in Sec. 1.1.2 which have an infinite set of conserved quantities but apparently only a few continuous symmetries, like translation in time or space. Note that the latter are the simplest type of symmetries on the form of Eq. (3.7) and they will be valid whenever the Lagrangian does not explicitly depend on these variables.

We now proceed to derive some conserved quantities for the continuum equation (3.1), starting with the invariance under translation in time. In terms of an infinitesimal transformation we write \( t \mapsto t + \epsilon \), i.e., \( T = 1 \) and \( X = \Upsilon = 0 \) in Eq. (3.7). By insertion in Eq. (3.9) we are led to the definition of the Hamiltonian density

\[
H = \frac{\partial L}{\partial \Psi_t} \Psi_t + \frac{\partial L}{\partial \Psi_t^*} \Psi_t^* - L = \frac{\alpha_1}{2} |\Psi|^2 - \frac{\alpha_2}{2} |\Psi_x|^2 + \frac{\alpha_3}{4} |\Psi|^4 - \alpha_4 (2|\Psi|^2|\Psi_x|^2 + 2|\Psi|^2 + |\Psi_x|^2) + c.c., \tag{3.11}
\]

and to the corresponding conserved quantity, the Hamiltonian \( H = \int H \, dx \). Since we arrive at the Hamiltonian by considering translations in time it is natural to identify this quantity with the total 'energy' of the system, but note that there is no guarantee that \( H \) is related to any physical energy in a real application. The current density associated with \( H \) is called the Hamiltonian flux density and is
from Eq. (3.10) given by

\[ J^{(H)} = 2 \text{Re} \{ \Psi_t^* \left[ \alpha_2 \Psi_x + 2\alpha_4 (\Psi^2 \Psi_x^* + 2|\Psi|^2 \Psi_x) \right] \} \]  

(3.12)

This will describe the flow of 'energy' in the system. From Eq. (3.5) and Eq. (3.11) it also follows that Eq. (3.1) and its complex conjugate can be derived from the Hamilton equations of motion, which will take the form

\begin{align*}
\frac{i}{\hbar} \Psi_t &= \frac{\partial H}{\partial \Psi^*} - \frac{d}{dx} \frac{\partial H}{\partial \Psi_x}, \\
\frac{i}{\hbar} \Psi_t^* &= \frac{\partial H}{\partial \Psi} - \frac{d}{dx} \frac{\partial H}{\partial \Psi_x^*}.
\end{align*}

(3.13a, 3.13b)

There is also an invariance under translations in space \( x \mapsto x + \epsilon, \) with \( X = 1 \) and \( T = \Upsilon = 0 \) in Eq. (3.7), and it is natural to call the corresponding conserved quantity, \( P = \int P \, dx, \) momentum. The momentum density is given by

\[ P = -\text{Im} \{ \Psi^* \Psi_x \}, \quad \text{(3.14)} \]

which together with the (scalar) momentum stress tensor from Eq. (3.10),

\[ J^{(P)} = \text{Im} \{ \Psi^* \Psi_t \} + \alpha_1 |\Psi|^2 + \alpha_2 |\Psi_x|^2 + \alpha_3 (\Psi^2 \Psi_x^* + \Psi^* \Psi_x^2 + 2|\Psi|^2 |\Psi_x|^2), \quad \text{(3.15)} \]

can be combined to a continuity equation. Although we have limited our discussion to one spatial dimension the momentum conservation is naturally generalized to more dimensions, where Eq. (3.14) will correspond to the \( x \) component of the momentum density vector. In two and three dimensions we may also expect the conservation of angular momentum. Here we note that \( \mathcal{L} \) in two spatial dimensions is invariant under the rotation

\[ x \mapsto \cos(\phi) x + \sin(\phi) y, \quad y \mapsto -\sin(\phi) x + \cos(\phi) y, \quad \text{(3.16)} \]

for \( \phi \in \mathbb{R}. \) Hence the infinitesimal rotation \( x \mapsto x + \epsilon y, \quad y \mapsto y - \epsilon x, \) will, through Noether's theorem, result in the conserved quantity \( M = \int M \, dx \, dy, \) with \( M = xP(y) - yP(x) = (\mathbf{r} \times \mathbf{P}) \cdot \mathbf{z}. \) The conservation law for general rotations in three dimensions is briefly covered in [107].

Further, changing the global phase of the complex field \( \Psi \) will not affect the dynamics of the system described by Eq. (3.1). The Lagrangian density (3.3), and hence the action integral (3.3), is invariant under the transformation \( \Psi \mapsto \Psi e^{i\phi}, \) \( \phi \in \mathbb{R}. \) Since this will also hold for infinitesimal phases, Noether's theorem is applicable with the transformation \( \Psi \mapsto \Psi + i\epsilon \Psi, \) i.e., \( \Upsilon = i\Psi \) and \( X = T = 0. \) The corresponding conserved quantity is called the norm, or excitation number,

\[ N = \int N \, dx, \quad \text{with norm density} \quad \mathcal{N} = |\Psi|^2 \quad \text{(3.17)} \]

In principle, a current density should not depend on quantities differentiated with respect to time, but the dependence on \( \Psi_t \) in Eq. (3.12) can be eliminated by the use of Eq. (3.1).
and norm current density

\[ \mathcal{J}^{(N)} = -2 \text{Im} \left\{ \alpha_2 \Psi_x \Psi^* + \alpha_4 (\Psi^2)_x \Psi^* \right\} \]

\[ = (\alpha_2 + 2\alpha_4 |\Psi|^2) \mathcal{P}. \tag{3.18} \]

An interesting point is that the Hamiltonian flux density (3.12) and the norm current density (3.18) will have a simple relation when restricted to stationary fields in a rotating frame of reference. If \( \Psi(x, t) = \psi(x) e^{-i\Lambda t} \), it follows that \( \mathcal{J}^{(H)} = \Lambda \mathcal{J}^{(N)} \). Note also that due to the phase invariance no harmonics will be generated in Eq. (3.1) by a field of this form, despite the nonlinearities.

When \( \alpha_4 = 0 \) in Eq. (3.1), the equation is Galilean invariant, meaning that the transformation

\[ t \mapsto t, \]

\[ x \mapsto x + 2\alpha_2 \epsilon t, \]

\[ \Psi \mapsto \Psi e^{i(\epsilon x - \alpha_2 \epsilon^2 t)}, \tag{3.19} \]

with \( \epsilon \in \mathbb{R} \), will not alter the form of the equation. Essentially this means that a stationary solution can be boosted to a mobile solution. However, the action integral \( S \) is not invariant under the transformation (3.19). Thus it will not yield another conserved quantity [167].

### 3.1.2 Solitons

In the absence of the nonlinear dispersion \( (\alpha_4 = 0) \), Eq. (3.1) reduces to the cubic nonlinear Schrödinger (NLS) equation

\[ i\Psi_t = \Psi_{xx} \pm |\Psi|^2 \Psi, \tag{3.20} \]

where the equation is rescaled according to \( \Psi(x, t) \mapsto \sqrt{\alpha_3/\alpha_2} \Psi(x, \alpha_2 t) e^{-i\alpha_1 t} \). The sign of the nonlinear term is \( \text{sgn}(\alpha_3/\alpha_2) \), i.e., positive if \( \alpha_2 \) and \( \alpha_3 \) have the same sign. Note that the elimination of the three parameters is done by using the phase invariance and by rescaling time and amplitude. Rescaling also the space variable, the fourth parameter, \( \alpha_4 \), can be eliminated in the full equation (3.1). As noted in Sec. 1.1.2, Eq. (3.20) includes the first effects of dispersion and nonlinearity on a wave packet and has a range of physical applications for systems incorporating these effects. Examples are models for packets of hydrodynamic waves on deep water [23], the propagation of pulses in nonlinear optical materials [114], and in particular optical fibres [94], heat pulses in solids, plasma waves and more [182].

With a positive sign in Eq. (3.20), the equation is called focusing since the nonlinear term will tend to compress an already localized excitation. The exact balance with the dispersive term is obtained for the soliton shape

\[ \Psi(x, t) = A \text{sech}(\alpha x - \beta t), \]

\[ |\Psi|^2 = A^2, \]

\[ \mathcal{J}^{(N)} = -2\alpha A^2 \text{sech}(\alpha x - \beta t) \text{sech}'(\alpha x - \beta t). \]

The condition for soliton existence is

\[ \alpha / \beta = \text{const}. \]

With a negative sign, it is called defocusing.

### Notes

1. Actually we only need to cancel the last term in the \( \alpha_4 \) part of the equation for this transformation to be valid [156]. Note also that the phase of the solution is changed in the transformation. Still this symmetry is generally referred to as Galilean invariance.
Some properties of nonlinear Schrödinger equations

Figure 3.1. Intensity profile of some solitons for the NLS equation, the breather Eq. (3.21) for \( a = 1 \) (solid) and \( a = 0.5 \) (dashed), and the dark soliton Eq. (3.24) for \( a = 1 \) (dotted).

\[ \Psi(x, t) = \sqrt{2a} \text{sech}(ax) e^{-ia^2 t}, \]  
(3.21)

This solution is sometimes called a breather since it is stationary and oscillating, but can be transformed to a moving soliton by the Galilei transformation Eq. (3.19). An illustration of the wave profile can be found in Fig. 3.1. The solution (3.21) has a zero phase gradient, i.e., for fixed \( t \) the solution can always be transformed to real form by the global phase invariance. In fact, this will be true for any localized stationary solution of Eq. (3.1). If we assume that a stationary solution has a spatially varying phase \( \theta(x) \) it can be represented on the form \( \Psi(x, t) = \psi(x) e^{-i(\theta(x) + \Lambda t)} \), where \( \psi \) and \( \theta \) are real functions. From the conservation law for the norm,

\[ \frac{dN}{dt} + \frac{dJ(N)}{dx} = 0, \]  
(3.22)

it then follows that

\[ J(N) = (\alpha_2 + 2\alpha_4 \psi^2)\psi_x \theta_x = C, \]  
(3.23)

where \( C \) is a constant. For a localized solution, with tails going to zero, we must have \( C = 0 \) and the only possibility to fulfill the conservation law is then \( \theta(x) = \theta_0 \), i.e., the phase of the solution is not allowed to vary in space. For solutions not decaying to zero, \( C \neq 0 \) is possible and the phase may vary. An exhausting classification can be found in [198]. Note also that if we want to induce mobility of a stationary solution we actually apply a phase gradient (\( e^{ikx} \)) across its extent. This will correspond to giving the solution a Galilean boost, as seen from Eq. (3.19) with \( t = 0 \).

With a negative sign of the nonlinearity, the NLS equation (3.20) is referred to as defocusing, since the nonlinearity will act to spread a localized pulse. Nonetheless, a form of localization is possible as a dip in a constant non-zero background.

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5With the plane wave \( Ae^{i(kx - \omega t)} \), the linear dispersion relation of the NLS equation is \( \omega = -k^2 \leq 0 \). Since the breather has a frequency \( \omega_0 = \alpha^2 > 0 \) it will always avoid resonances with phonons. Sometimes the name NLS breather is reserved for the bound state of two solitons, which will have an oscillating intensity.

6But see also the comment in Chapter 4.
3.2 Discrete equations

The nonlinearity will act to compress the dip and the dispersion will act to spread it, thus forming a so-called dark soliton

\[ \Psi(x,t) = \sqrt{2a} \tanh(ax) e^{i4\pi^2 t}, \] (3.24)

which is depicted in Fig. 3.1.

Including the nonlinear dispersive terms in Eq. (3.1) there are also breather solutions. An implicit formula for their form is derived in paper II (see Eq. (15) and Fig. 2). This solution cannot in general be boosted to an exact moving soliton due to the lack of Galilean invariance of the general form of Eq. (3.1). The presence of the nonlinear dispersion can also lead to the existence of exotic solitons, again given by implicit formulas in paper II (Eqs. (15), (17) and (19)–(21) and Fig. 2). However, these will all suffer from some form of instability.

3.2 Discrete equations

The main equation studied in this thesis is the discrete nonlinear Schrödinger (DNLS) equation with nonlinear coupling that was derived in two different contexts in the preceding chapter (Eqs. (2.26) and (2.41)) and for special parameter values as a rotating-wave approximation of the dynamics in an FPU lattice (Eq. (1.45)),

\[ i \frac{d\Psi_m}{dt} = Q_1 \Psi_m + Q_2 (\Psi_{m-1} + \Psi_{m+1}) + 2Q_3 \Psi_m |\Psi_m|^2 
+ 2Q_4 [2\Psi_m (|\Psi_{m-1}|^2 + |\Psi_{m+1}|^2) + \Psi_m^* (\Psi_{m-1}^2 + \Psi_{m+1}^2)] 
+ 2Q_5 [2|\Psi_m|^2 (\Psi_{m-1} + \Psi_{m+1}) + \Psi_m^2 (\Psi_{m-1}^* + \Psi_{m+1}^*) 
+ \Psi_{m-1} |\Psi_{m-1}|^2 + \Psi_{m+1} |\Psi_{m+1}|^2]. \] (3.25)

The number of independent parameters of Eq. (3.25) can be reduced to two by rescaling amplitude and time, and by using the global phase invariance to get rid of the parameter \( Q_1 \) with the transformation \( \Psi_m(t) \mapsto \Psi_m(t)e^{-iQ_1 t} \). An extensive investigation of the discrete equation is therefore necessarily more elaborate than for the continuum equation (3.1), where all parameters could be eliminated and the solutions essentially only are parameterized by dynamical parameters, like norm, or spectral parameters, like frequency and velocity. Some restriction on the parameter space for Eq. (3.25) is possible since the staggering transformation \( \Psi_m \mapsto (-1)^m \Psi_m \) is equivalent to the change of parameters \( Q_2 \mapsto -Q_2 \) and \( Q_5 \mapsto -Q_5 \).

The discrete equation has some symmetries similar to those for the continuum equation, while others are destroyed by the discreteness. For a Lagrangian formulation of Eq. (3.25), instead of the field variables \( \Psi \) and \( i\Psi^* \), the sets \( \{\Psi_m\} \) and \( \{i\Psi_m^*\} \) are required. Variation of the action integral (3.3) with respect to these

---

7See also [113] for some examples of grey solitons, having a nonzero minimum intensity and a spatially varying phase.
Some properties of nonlinear Schrödinger equations

variables gives
\[
\frac{\delta S}{\delta \Psi_m} = 0 \iff \frac{\partial L}{\partial \Psi_m} - \frac{d}{dt} \frac{\partial L}{\partial \Psi_{m,t}} = 0, \tag{3.26a}
\]
\[
\frac{\delta S}{\delta \Psi_m^*} = 0 \iff \frac{\partial L}{\partial \Psi_m^*} - \frac{d}{dt} \frac{\partial L}{\partial \Psi_{m,t}} = 0, \tag{3.26b}
\]
where \( \Psi_{m,t} = d\Psi_m/dt \). Working our way backwards we see that Eq. \[(3.25)\] will be produced by the Lagrangian \( \mathcal{L} = \sum_m \mathcal{L}_m \), with Lagrangian density
\[
\mathcal{L}_m = \frac{i}{2} \Psi^*_m \Psi_{m,t} - \frac{Q_1}{2} |\Psi_m|^2 - \frac{Q_2}{2} \Psi_m \Psi^*_m \Psi_{m+1} - \frac{Q_3}{2} |\Psi_m|^4 - Q_4 (2|\Psi_m|^2|\Psi_{m+1}|^2)
+ \Psi^2_m \Psi^2_{m+1} - 2Q_5 \Psi_m \Psi_{m+1} (\Psi^2_m + \Psi^2_{m+1}) + c.c.. \tag{3.27}
\]
The Lagrangian density is not uniquely defined, but the Lagrangian \( \mathcal{L} \) is, at least up to trivial terms of the form \( \text{Re}\{\Psi_m\Psi_{m,t}\} \). \( \mathcal{L}_m \) is just a decomposition of this quantity. The dependence in Eq. \[(3.27)\] is just a symmetric grouping of terms depending on \( \Psi_m, \Psi_{m+1} \) and their complex conjugates. In principle other densities can be defined as long as they add up to the Lagrangian, but the definition Eq. \[(3.27)\] will prove to be convenient.

### 3.2.1 Symmetries and conserved quantities

In the discrete version of Noether’s theorem we consider infinitesimal transformations, under which the action integral \( S \) is invariant, on the form
\[
t \mapsto t + \epsilon T, \\
\Psi_m \mapsto \Psi_m + \epsilon \Upsilon_m, \tag{3.28}
\]
where \( T \) and \( \Upsilon_m \) are functions of \( t, \Psi_n \) and \( \Psi_{n,t} \) for \( n \in \mathbb{Z} \). The conserved quantity corresponding to this symmetry is
\[
I = \sum_n \frac{\partial L}{\partial \Psi_{n,t}} (\Psi_{n,t} T - \Upsilon_n) + \sum_n \frac{\partial L}{\partial \Psi_{n,t}^*} (\Psi_{n,t}^* T - \Upsilon_n^*) - LT, \tag{3.29}
\]
i.e., \( dl/dt = 0 \). A proof can be found in \[(3.25)\]. The conserved quantities of the discrete equation \[(3.25)\] are now readily derived. The invariance under translation in time \( t \mapsto t + \epsilon \), i.e., \( T = 1 \) and \( \Upsilon_m = 0 \), leads to a conservation of Hamiltonian, which by the decomposition of Eq. \[(3.27)\] may be written as a sum over a Hamiltonian density \( \mathcal{H} = \sum_m \mathcal{H}_m \),
\[
\mathcal{H}_m = \frac{\partial \mathcal{L}_m \Psi_{m,t}}{\Psi_{m,t}} + \frac{\partial \mathcal{L}_m \Psi_{m,t}^*}{\Psi_{m,t}^*} - \mathcal{L}_m
= \frac{Q_1}{2} |\Psi_m|^2 + \frac{Q_2}{2} \Psi_m \Psi^*_m \Psi_{m+1} + \frac{Q_3}{2} |\Psi_m|^4 + Q_4 (2|\Psi_m|^2|\Psi_{m+1}|^2)
+ \Psi^2_m \Psi^2_{m+1} - 2Q_5 \Psi_m \Psi_{m+1} (\Psi^2_m + \Psi^2_{m+1}) + c.c.. \tag{3.30}
\]
Further, a set of the Hamilton equations of motion can be derived for the given Hamiltonian. From Eq. (3.26) it follows that

\[ \frac{d\Psi_m}{dt} = \frac{\partial H}{\partial \Psi_m} \],  

(3.31a)

\[ -\frac{d\Psi_m^*}{dt} = \frac{\partial H}{\partial \Psi_m} \],  

(3.31b)

will yield Eq. (3.25) and its complex conjugate.

There is also an invariance under global phase rotations, i.e., the transformation \( \Psi_m \mapsto \Psi_m e^{i\phi}, \phi \in \mathbb{R} \), will have no effect on the properties of the system. For infinitesimal rotations this is a transformation on the form of Eq. (3.28), with \( T = 0 \) and \( \Upsilon_m = i\Psi_m \). Hence from Noether’s theorem there is a conserved quantity, the norm (or excitation number),

\[ N = \sum_m N_m = \sum_m |\Psi_m|^2. \]  

(3.32)

In our physical applications the norm will in the waveguide context correspond to conservation of Poynting power as the electric fields propagate along the array, and in the case of coupled Bose-Einstein condensates it will represent boson number conservation.

The discrete equation (3.25) is, just as the continuum equation (3.1), invariant under spatial translations. However, due to the discreteness such a transformation is given by \( m \mapsto m + k \), where \( m \) refers to a site and \( k \in \mathbb{Z} \). Although this transformation leaves the action integral unchanged for any integer \( k \), Noether’s theorem cannot be applied since this is not a continuous symmetry. Thus momentum, and angular momentum in more spatial dimensions, are not conserved due to the lattice discreteness.

For the discrete equation, Noether’s theorem does not provide any continuity equations, only the conserved quantities. Nonetheless, it is possible to express the conservation laws as discrete continuity equations. With the Lagrangian written as a sum over a Lagrangian density, \( L = \sum_m \mathcal{L}_m \), the conserved quantity given by Eq. (3.29) can be written on the form \( \mathcal{I} = \sum_m I_m \). An appropriately chosen current density \( J_m \) will by this division provide a discrete continuity equation

\[ \frac{dI_m}{dt} + J_m - J_{m-1} = 0, \]  

(3.33)

from the conservation law \( d\mathcal{I}/dt = 0 \). Note that the form of the continuity equation is not unique, since the decomposition of the Lagrangian is not unique. However, by letting \( \mathcal{L}_m \), and consequently \( \mathcal{I}_m \), be a function of \( \Psi_m \) and \( \Psi_{m+1} \), the current density \( J_m \) can be chosen to depend only on the same variables. Thus we are led to the very reasonable interpretation of \( J_m \) as the current flowing from site \( m \) to site \( m + 1 \) of the lattice.

---

8Note that the spatial variable \( z \), which measures the distance along the waveguides, will play the role of time in this formulation (see chapter 2).
To derive a continuity equation for the Hamiltonian we start out by differentiating the Hamiltonian density \((3.30)\) with respect to time. The result is

\[
\frac{d\mathcal{H}_m}{dt} = \frac{\partial\mathcal{H}_m}{\partial\Psi_{m+1}} \frac{d\Psi_{m+1}}{dt} + \frac{\partial\mathcal{H}_m}{\partial\Psi_{m}} \frac{d\Psi_{m}}{dt} + \text{c.c.}
\]

\[
= \frac{\partial\mathcal{H}_m}{\partial\Psi_{m+1}} \frac{d\Psi_{m+1}}{dt} + \left( -\frac{\partial\mathcal{H}_{m-1}}{\partial\Psi_{m}} - i\frac{d\Psi_{m}^{\ast}}{dt}\right) \frac{d\Psi_{m}}{dt} + \text{c.c.} \quad (3.34)
\]

where Eq. \((3.31b)\) has been used together with the assumption that \(\mathcal{H}_m\) only depends on \(\Psi_{m}, \Psi_{m+1}\) and their complex conjugates. It is now natural to define the Hamiltonian flux density as

\[
\mathcal{J}^{(H)}_m = -2\text{Re} \left\{ \frac{d\Psi_{m+1}}{dt} \frac{\partial\mathcal{H}_m}{\partial\Psi_{m+1}} \right\}
\]

\[
= -2\text{Re} \left\{ \frac{\partial\Psi_{m+1}}{\partial\Psi_{m+1}} \left[ Q_2\Psi_{m} + 2Q_4\Psi_{m}^{\ast}(2\Psi_{m}\Psi_{m+1}^{\ast} + \Psi_{m}^{\ast}\Psi_{m+1}) \right] 
\]

\[
+ 2Q_5\left( \Psi_{m}(\Psi_{m}^{\ast2} + \Psi_{m+1}^{\ast2}) + 2\Psi_{m}^{\ast}\Psi_{m+1}|\Psi_{m+1}|^2 \right) \right\}.
\]

Similarly, a continuity equation for the norm can be derived. A very nice way of doing this is by making a transformation to action-angle variables by setting \(\Psi_m(t) = \sqrt{N_m}e^{-i\theta_m(t)}\). This is a canonical transformation and the dynamics of Eq. \((3.25)\) is equally well described by an alternative set of the Hamilton equations of motion \([87, 155]\)

\[
\frac{d\theta_m}{dt} = \frac{\partial\mathcal{H}}{\partial N_{m}},
\]

\[
-\frac{dN_{m}}{dt} = \frac{\partial\mathcal{H}}{\partial \theta_m}. \quad (3.36a, 3.36b)
\]

Since Eq. \((3.36b)\) contains the derivative of the norm density \(N_{m} = |\Psi_{m}|^2\) with respect to time, it is now straightforward to derive a continuity equation. Introducing \(\phi_{m+1} = \theta_{m+1} - \theta_m\) for the phase difference between neighbouring sites we get

\[
\frac{dN_{m}}{dt} = -\frac{\partial}{\partial \theta_m} \sum_n \mathcal{H}_n = -\frac{\partial\mathcal{H}_m}{\partial \phi_{m+1}} \frac{\partial\phi_{m+1}}{\partial \theta_m} - \frac{\partial\mathcal{H}_{m-1}}{\partial \phi_m} \frac{\partial\phi_m}{\partial \theta_m}
\]

\[
= \frac{\partial\mathcal{H}_m}{\partial \phi_{m+1}} - \frac{\partial\mathcal{H}_{m-1}}{\partial \phi_m}.
\]

\text{Note that there is really no controversy in the definition of the norm density. This is the only sensible decomposition of the norm \(N\), especially since we in our physical applications can identify the norm density with the power in one specific waveguide or the number of bosons in one specific potential well.}
Thus, with the decomposition of the Hamiltonian in Eq. (3.30) we see that the flow of norm in the lattice is intimately linked to the phase difference of neighbouring sites, and we define the norm current density

$$J_m^{(N)} = -\frac{\partial H_m}{\partial \phi_{m+1}} = 2\sqrt{N_m N_{m+1}} \sin \phi_{m+1} \times \left[ Q_2 + 4Q_4 \sqrt{N_m N_{m+1}} \cos \phi_{m+1} + 2Q_5 (N_m + N_{m+1}) \right]$$

(3.38)

Some effects of the nontrivial dependence of this quantity on the phase difference between neighbouring sites are addressed in Sec. 3.2.3 and also presented in paper III for the one-dimensional model and in paper V for the two-dimensional model. The generalization of the continuity equation (3.33) to higher spatial dimensions is trivial and an example with the norm is given in paper V.

### 3.2.2 Discrete breathers

In Sec. 1.2 many of the general properties of DBs were briefly discussed. In this section, and the following, we will recapitulate some of these results for the solutions of the DNLS equations and also expand on some specific topics. The most widely studied form of this class of equations is the cubic DNLS equation, i.e., Eq. (3.25) with $Q_4 = Q_5 = 0$. Apart from being a generic equation for systems with coupling and nonlinearity (Sec. 1.2.4), it is also a model in its own right for many systems. Examples are models for polarons in molecular crystals [96], (Davydov) solitons on proteins [184], nonlinear photonic crystals [148] and, of interest for this thesis, coupled nonlinear optical waveguides (Sec. 2.1.5) and Bose-Einstein condensates in periodic potentials (Sec. 2.2). For a review of the DNLS equation see [62]. Different extensions of this model have been suggested to study, e.g., forms of the nonlinearity other than the cubic, or long-range interactions beyond the nearest-neighbour coupling. Here we are strictly interested in the additional effects from a nonlinear coupling.

To find localized solutions of Eq. (3.25) we can employ the method of continuation from the anti-continuous limit, previously mentioned in Sec. 1.2.2. Setting $Q_2 = Q_4 = Q_5 = 0$ will result in a system of uncoupled anharmonic oscillators,

$$i \frac{d \Psi_m}{dt} = Q_1 \Psi_m + 2Q_3 \Psi_m |\Psi_m|^2,$$

(3.39)

the solution of which is trivial,

$$\Psi_m(t) = \sqrt{\frac{\Lambda_m}{2Q_3}} e^{-i[(\Lambda_m + Q_1)t + \theta_m]}.$$

(3.40)

The frequencies $\Lambda_m$ and phases $\theta_m$ can be chosen arbitrarily and independently for each site. However, due to restrictions set by the discrete continuity equations,
Some properties of nonlinear Schrödinger equations

not all possible configurations will survive continuation to nonzero coupling. If we only are interested in stationary solutions, i.e., solutions with constant intensity \( N_m = |\Psi_m|^2 \), the continuity equation for the norm,

\[
\frac{dN_m}{dt} + J_m^{(N)} - J_{m-1}^{(N)} = 0,
\]

will reduce to the conservation law \( J_m^{(N)} = J_{m-1}^{(N)} \), with the norm current density given by Eq. (3.38). If the solution is localized we must further require that \( J_m^{(N)} = 0 \). As a consequence the phase difference between neighbouring sites must in the absence of nonlinear coupling \( (Q_1 = 0) \) satisfy \( \phi_{m+1} = \theta_{m+1} - \theta_m \in \{0, \pi\} \).

In extension, this result implies that any stationary solution with a finite number of excited sites not forming a closed loop in the anti-continuous limit must have this trivial relation between phases. Without restriction, the global phase invariance will allow us to consider only real solutions in this instance. An ansatz with real amplitudes,

\[
\Psi_m(t) = \psi_m e^{-i(A + Q_1) t}
\]

will reduce Eq. (3.26) to an algebraic equation,

\[
\Lambda \psi_m = Q_2 (\psi_{m-1} + \psi_{m+1}) + 2Q_3 \psi_m^3 + 6Q_4 \psi_m (\psi_{m-1}^2 + \psi_{m+1}^2) + 2Q_5 \left[ 3 \psi_m^2 (\psi_{m-1} + \psi_{m+1}) + \psi_{m-1}^3 + \psi_{m+1}^3 \right],
\]

with solutions \( \psi_m \in \{0, \pm \sqrt{\Lambda/2Q_2}\} \) at the anti-continuous limit. For continuation to nonzero coupling we must also be sure that \( \Lambda \) is nonresonant with the phonons of the system. Here we have a single-frequency solution, but for a general time-periodic solution none of the harmonics may resonate with the linear spectrum. In the anti-continuous limit of Eq. (3.39) this means that \( n(\Lambda + Q_1) \neq Q_1, n \in \mathbb{Z} \), which can be written as \( \Lambda/Q_1 \neq (1 - n)/n \). Thus it appears as if there may be a resonance for some frequencies. However, the phase invariance of Eq. (3.26) means that \( Q_1 \) essentially is an arbitrary parameter that can be changed by switching to a rotating frame of reference. The transformation \( \Psi_m \mapsto \Psi_m e^{-iA_0 t} \) in the original equation (3.26) is equivalent to the change \( Q_1 \mapsto Q_1 - \Lambda_0 \). The nonresonance condition will thus transform to \( \Lambda/(Q_1 - \Lambda_0) \neq (1 - n)/n \). Since \( \Lambda_0 \) is arbitrary, the phase invariance makes the nonresonance condition an artificial condition for the time-periodic solutions of the DNLS equations, that can be worked around by changing reference frame.

Just as discussed in Sec. 1.2.2 the configuration at the anti-continuous limit can be used to label the solutions. Choosing to excite only a few sites at this limit will by continuation lead to exponentially localized excitations in the lattice

\[\text{[10]}\]

A closed loop can be formed if the system has periodic boundary conditions or in the form of vortices in higher dimension. For excitations located \( k \) sites apart the strength of their interaction through the linear coupling will be of order \( Q_k^2 \), but the phase relation must still hold. This is demonstrated in [102] where the phase condition for the DNLS equation also is discussed for non-stationary solutions.

\[\text{[11]}\]

Note that \( \Lambda + Q_1 \) is still the frequency of the DB in the original reference frame, i.e., oscillations with this frequency will occur if a site with amplitude \( \sqrt{\Lambda/2Q_2} \) is excited and evolved according to Eq. (3.26).
for finite coupling. Numerically this can be done by taking the exact solution
for zero coupling as initial condition in a Newton iteration of Eq. (3.43) with
the coupling slightly turned on. When the method has converged the coupling
is increased again and a new solution found with the previous solution as an
initial guess. This method was described in Sec. 1.2.3. In this continuation we
may, e.g., take the spectral parameter $\Lambda$ as a fixed parameter and obtain DBs
for varying coupling. Changing $\Lambda$ will instead generate a family of solutions for
fixed coupling.\footnote{For the DNLS equation ($Q_4 = Q_5 = 0$) rescalings reveal that
the nonlinearity can be fixed in strength and the relevant physical properties can be
expressed in the parameter $Q_2/\Lambda$.} Alternatively, the continuation may be considered under the
constraint of fixed norm $N$ and the frequency allowed to vary with the coupling.
This is advantageous if we are interested in the connection between the stationary
solutions and mobile solutions, since $N$ is a conserved quantity (see Sec. 1.2.6).
In this case the set of equations (3.43) are supplemented with the constraint $N -
\sum_m \psi_m^2 = 0$. The extra equation means that we need an extra variable, and the
frequency $\Lambda$ must now be treated as an unknown quantity (a Lagrange multiplier)
to be solved for. With this extension the simplified method for stationary solutions
described in Sec. 1.2.3 can still be used.

With these methods it is easy to calculate stationary solutions of the DNLS
equation. The most fundamental modes are the site-centred solution, with a single
site excited in the uncoupled limit, and the symmetric and anti-symmetric bond-
centred solutions, with two neighbouring sites excited. The spatial forms of these
modes were exemplified in Fig. 1.4. Further, the linear stability of the solutions
can be investigated using the method described in Sec. 1.2.3. The distribution of
the eigenvalues as a function of their norm is shown in Fig. 3.2 for the two most
fundamental modes, in the case of a focusing nonlinearity for the cubic DNLS
equation with $Q_2 = 0.2$, $Q_3 = 0.5$ and $Q_4 = Q_5 = 0$.\footnote{The solutions will have an unstaggered tail, cf. Fig. 1.4.} The site-centred solution
is always stable, while the symmetric bond-centred solution always is unstable.
The positive eigenvalue that approaches the imaginary axis for the two-site DB in
Fig. 3.2c only asymptotically goes to zero as the norm is decreased. In the low norm
limit, which also corresponds to low frequencies in this case, the solutions are close
to the continuum limit, where the system can be described by the focusing NLS
equation (3.20), and the two DBs degenerate into the NLS soliton, Eq. (3.21). The unstable mode for the two-site solution, and the mode approaching the origin along
the imaginary axis for the one-site solution (seen around $N = 0.5$ in Fig. 3.2c),
will in the continuum limit correspond to a translational mode with eigenvalue zero.
This internal mode is thus connected to the continuous translational symmetry of
the continuum equation. The mode is symmetry-breaking and its excitation will
lead to soliton motion in the continuous system. It is similar to the depinning modes
with zero eigenvalue discussed in Sec. 1.2.6 for discrete systems. However,
for the cubic DNLS equation there will be no depinning modes since there is no
change of the stability of the fundamental modes. The mobility of DBs in this
model is also very poor away from the continuum limit. The third fundamental
mode, the anti-symmetric bond-centred solution with an unstaggered tail will for
the given parameter values exist for $N \geq 1.914$ and be stable for $N \geq 3.946$. It
Some properties of nonlinear Schrödinger equations

Figure 3.2. The eigenvalue spectrum of solutions for the cubic DNLS equation with $Q_2 = 0.2, Q_3 = 0.5$ ($Q_4 = Q_5 = 0$) as function of the norm. (a) and (b): the site-centred solution. (c) and (d): the symmetric bond-centred solution. The spectra of extended eigenmodes are clearly seen as the bands in the plots for the imaginary part. From (a) we see that the site-centred solution is stable, while (c) shows that the bond-centred solution is unstable (the eigenvalue only asymptotically goes to zero). Periodic boundary conditions on a lattice with 201 sites were used in the calculations.

cannot exist for small values of the norm since the phase difference of $\pi$ between its main excited sites has no correspondence in the continuum limit. A more exhaustive investigation of the stability of various DBs of the cubic DNLS equation and their connections through bifurcations can be found in [39, 64, 65] (only systems with up to six sites are studied).

For the corresponding two-dimensional model there will be an excitation threshold for localized solutions, i.e., they will only exist above some critical value of the norm [146, 201]. It can be shown that the one-site solution will be stable for high frequencies, but it will become unstable for low frequencies [124]. In the latter case the solution is close to the continuum limit and the unstable soliton of the two-dimensional cubic DNLS equation. Solutions with two sites excited in the anti-continuous limit are generally unstable, but the anti-symmetric DB (if the tail is unstaggered) can be stable for high frequencies (or high norm).

With the inclusion of nonlinear coupling ($Q_4, Q_5 \neq 0$) the issue of stability of the fundamental modes will be more complex both in the one- and two-dimensional models. For example, there will be an exchange of stability between the fundamen-
3.2 Discrete equations

Figure 3.3. Exotic DBs of Eq. (3.29). (a) Three-site compact DB, here with all excited sites of the same amplitude $\Psi_m = \sqrt{-Q_2/2Q_5} = 1$ and frequency $\Lambda = -Q_2Q_4/Q_5 = 1$ ($Q_2 = 1$, $Q_3 = 0.5$, $Q_4 = 0.5$, $Q_5 = -0.5$). This configuration is unstable. (b) A stable DB with a single phase twist at the center ($\cos \phi = -5/6$) and frequency $\Lambda = 3.0495$. The real (imaginary) parts are indicated by filled (unfilled) circles ($Q_2 = 1$, $Q_3 = 0.5$, $Q_4 = 0.01$, $Q_5 = -0.1$).

tal modes that is connected to the existence of intermediate solutions, as discussed in Sec. 1.2.6. The connection of this phenomenon to DB mobility is investigated in papers I and V. Another intriguing effect of the nonlinear coupling is the compactification of localized solutions. For certain parameter values DBs can exist without an exponentially decaying tail. This is possible when the linear and nonlinear coupling are of opposite signs, since this can lead to a total coupling between lattice sites that is zero and a subsequent decoupling of the lattice between these sites (Sec. 1.2.7). For the stationary solutions of Eq. (3.43) an $M$-site compact DB is an excitation that for some site $k$ fulfills $\psi_{k+j} = 0$ for $j \leq -1$ and $j \geq M$, and $\psi_{k+j} \neq 0$ for $j = 0, 1, \ldots, M - 1$. From the equation at site $m = k - 1$ we then get

$$Q_2 + 2Q_5\psi_k^2 = 0,$$

and similarly for the site $m = k + M$. As Eq. (3.44) describes the effective coupling between sites $k-1$ and $k$ it is possible, if $Q_2$ and $Q_5$ have opposite signs, to choose the amplitude so that the lattice is essentially decoupled into an excited portion and resting portions. Note that Eq. (3.44) is a general criterion that implies the existence of compact DBs with any number of sites $M$. The criterion will be the same in two dimensions, although it must be fulfilled for more nearest neighbours. Fig. 3.4 illustrates a three-site compact solution in the one-dimensional model. Examples, and explicit formulas for the form of compact solutions, can also be found in papers I, III and V. Observe that the solutions are only compact within the model (3.29). In a physical setting, e.g., an array of coupled optical waveguides, Eq. (3.29) describes the amplitudes of the propagating modes of the electric field in each waveguide. These modes are themselves spatially exponentially localized, see, e.g., the solutions for the modes in Appendix A. Thus, measurements will always at most yield exponential localization. The compact solutions will however represent the most extreme form of localization possible in this context.
3.2.3 Stationary solutions with nontrivial phase

When we in Sec. 3.2.2 made a reduction of stationary solutions to real solutions, i.e., solutions that are real in some rotating frame of reference, we made two restrictions to ensure the vanishing of the norm current. The first was to consider systems without nonlinear coupling and the second was that the excited sites should not form a closed loop.

Lifting the first restriction implies that the phase difference between neighbouring sites no longer needs to be 0 or \( \pi \). For a localized solution we must still require that the norm current density \( J_{m}^{(N)} \) vanishes, but from Eq. (3.11) there is now the additional zero

\[
\cos \phi_{m+1} = -\frac{Q_{2} + 2Q_{5}(N_{m} + N_{m+1})}{4Q_{4}\sqrt{N_{m}N_{m+1}}}. \tag{3.45}
\]

Thus, with nonlinear coupling localized stationary solutions can be complex. The effects of this property was first published with paper [III] and the extension to two dimensions was considered in paper [V]. An example of a linearly stable solution with a single phase twist is shown in Fig. 3.3b. It is important to underline that these solutions are stationary, despite the nontrivial phase. In general a phase twist is associated with a transport of norm, but, as shown with Eq. (3.45), the nonlinear coupling can halt this transfer. Further, in view of the compact solutions discussed in Sec. 3.2.2, the phase twisted solutions can also be compact. Explicit examples with two excited sites can be found in paper [III] and more examples are found in paper [V].

Lifting instead the second restriction, we are interested in stationary solutions whose excited sites form closed loops. In a one-dimensional system this is only possible with periodic boundary conditions and an excitation that extends over the entire system, i.e., a plane wave. The plane wave solution will be stationary, i.e., its intensity will not change, but it still represents a transport of norm (and Hamiltonian) in the system. Since this solution is not localized the continuity equation for the norm, Eq. (3.11), will now only reduce to the conservation law \( J_{m}^{(N)} \equiv J_{m}^{(N)} = J_{m-1}^{(N)} \), which is only an expression of the fact that the flow of norm is balanced for each site. With the ansatz \( \Psi_{m} = \sqrt{\rho} e^{-i(\phi_{m} + \Lambda t)} \) in Eq. (3.25) the norm current is

\[
J_{m}^{(N)} = 2\rho \sin \phi [Q_{2} + 4Q_{4}\rho \cos \phi + 4Q_{5}\rho]. \tag{3.46}
\]

A similar relation will hold also in two dimensions, where Eq. (3.46) will be the current flowing in each lattice direction and \( \phi \) will be the phase gradient (wave number) along that direction. The frequency \( \Lambda \) can be obtained from Eq. (3.25), but it can also be directly calculated from the Hamiltonian density \( H_{m} \) in Eq. (3.30).

From the Hamilton equations of motion in action-angle variables, Eq. (3.36a), we get

\[
\frac{d\theta_{m}}{dt} = \frac{\partial}{\partial N_{m}} \sum_{n} \mathcal{H}_{n} = \frac{\partial \mathcal{H}_{m-1}}{\partial N_{m}} + \frac{\partial \mathcal{H}_{m}}{\partial N_{m}}, \tag{3.47}
\]
With a constant-amplitude solution $N_m = \rho$ and a rotating phase with constant phase gradient, $\theta_m = \phi m + \Lambda t$, the frequency is given by

$$\Lambda = \frac{\partial H_m}{\partial \rho} = Q_1 + 2(Q_2 + 8Q_3) \cos \phi + 2Q_3 \rho + 4Q_4 \rho (2 + \cos 2\phi), \tag{3.48}$$

where we have used that $H_m$ is symmetric with respect to the interchange $m \leftrightarrow m + 1$. The relation is a special case of the more general relation $\Lambda = dH/dN$ for stationary solutions. A very interesting effect involving the nonlinear coupling is the additional zero, Eq. (3.45), of the norm current. Since the zero depends on the amplitude $\rho$ of the plane wave it means that for a given phase gradient $\phi$ the amplitude can be tuned to make the norm current zero. Moreover, when the amplitude is varied past the zero, the direction of the current will be reversed. This means that the flow of norm across the lattice, which corresponds to power flow for coupled optical waveguides, can be controlled in detail. A prerequisite for this control is that the plane waves are stable in the range over which the amplitude is varied. The stability can in the interesting cases be confirmed with the technique presented in Sec. 1.2.4, where a small modulation is added as a perturbation to the plane wave. The details are presented in paper [11] and extended to two dimensions, showing an even greater flexibility than in one dimension, in paper [V]. Of course, in two dimensions it is hard to imagine an array of waveguides with periodic boundary conditions in both directions, while in one dimension we simply put the waveguides in a ring. However, if there is a supply of power along one boundary and a drain of power along the other boundary, the plane wave solutions can be sustained also without periodic boundary conditions.

To form a closed loop for the norm current in the interior of a lattice we need at least two dimensions. Such solutions can be constructed from the anti-continuous limit by taking a configuration with excited sites oriented along some contour in the lattice forming a closed loop. If all sites are chosen with the same amplitude and phase this will be a multisite DB. We can also choose the excited sites to have the same amplitude, but different phases. In this case there will in general be a flow of norm along the contour, but as long as the flow is balanced for each site the solution will still be stationary also for finite coupling. However, we must require that the overall phase change for one complete turn around the contour is a multiple of $2\pi$. The number of $2\pi$ phase twists, $S$, is called the topological charge, or vorticity, of the excitation. The most simple excitation carrying topological charge is a vortex with four excited sites in the anti-continuous limit and a phase difference of $\pi/2$ between sites. This, and other configurations, are listed in paper [V], where also a short review of some results on vortices in DNLS models is given in the introduction. The main result of this paper is the existence of a stable vortex with topological charge $S = 2$, previously not thought to exist for the cubic DNLS model. The topological charge is proportional to the angular momentum carried by the vortex, but due to the discreteness of the lattice this is not a conserved quantity (Sec. 3.2.1). Thus, when a vortex is destroyed, the vorticity is generally not conserved. Moreover, as with the other forms of excitations, the inclusion of nonlinear coupling can lead to compact discrete vortices (paper [V]).
3.2.4 Quasiperiodic solutions

From the trivial solution, Eq. (3.40), at the anti-continuous limit of Eq. (3.25) we see that different frequencies, and thus amplitudes, can be chosen for different sites. If sites are excited with two different incommensurate frequencies $\Lambda_1$ and $\Lambda_2$, the resulting solution will not be periodic [102, 103, 133]. A condition for the existence of the solution outside the anti-continuous limit is still that resonances with the linear spectrum must be avoided. As soon as there is coupling between the sites in the lattice the frequencies will mix and any linear combination of the two frequencies will be present. Thus the nonresonance condition for Eq. (3.39) must be stated as

$$n_1(\Lambda_1 + Q_1) + n_2(\Lambda_2 + Q_1) \neq Q_1,$$

where $n_1, n_2 \in \mathbb{Z}$. Since the mixed harmonics densely fill the real line for incommensurate frequencies the continuation to nonzero coupling would in general be impossible. However, as discussed above, resonances with the linear spectrum can be avoided by changing to a rotating frame of reference. Thus the condition can be transformed to

$$n_1(\Lambda_1 + (Q_1 - \Lambda_0)) + n_2(\Lambda_2 + (Q_1 - \Lambda_0)) \neq Q_1 - \Lambda_0.$$ 

In particular it will be fulfilled for incommensurate frequencies, and quasiperiodic solutions will always exist for finite coupling. Further, in the rotating frame of reference the two different types of excited sites in the anti-continuous limit now be either constant or oscillating with the frequency $\Lambda_b = \Lambda_2 - \Lambda_1$. For finite coupling such a solution cannot be stationary, nor can it be transformed to real form by use of the global phase invariance. Since there is a time-dependent phase difference between the sites excited with different amplitudes, there will be a periodic flow of norm between the sites and the intensity of the quasiperiodic DB will oscillate with the frequency $\Lambda_b$. Note that the above discussion is independent of the lattice dimension and quasiperiodic solutions will also exist in arbitrary dimension for the DNLS equations [104]. Note also that it is not possible to have solutions with three, or more, incommensurate frequencies since the nonresonance condition cannot be fulfilled in any reference frame in this case.

To numerically find quasiperiodic solutions the general iterative method described in Sec. 1.2.3 can be used. The idea is to work in the reference frame rotating with frequency $\Lambda_1$ so that the solution we are seeking is periodic with frequency $\Lambda_b = \Lambda_2 - \Lambda_1$. Using this method, quasiperiodic solutions were computed for the one-dimensional cubic DNLS model in [102]. Some of the simplest quasiperiodic configurations, e.g., two neighbouring sites with different amplitude at the anti-continuous limit, were also shown to be linearly stable for small coupling. In general, a necessary condition for stability is $n\Lambda_1 \neq 2\Lambda_1$, $n \in \mathbb{Z}$ (see [102] for more details). In two dimensions stable solutions have also been calculated [104]. An example of a quasiperiodic vortex can be found in paper IV, where it is shown that charge flipping, i.e., when the topological charge of a vortex periodically changes between $S$ and $-S$, is connected to quasiperiodic excitations in the lattice.

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14Note that if we write down the nonresonance condition directly in the frame rotating with frequency $\Lambda_1$, we are lead to $n(\Lambda_2 - \Lambda_1) = n\Lambda_b \neq \Lambda_1$. This is equivalent to the derived condition for $n = -n_2$. 

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Comments and conclusion

In Part II, the main results of the thesis work is presented in five papers. A selection of results has briefly been mentioned in the previous chapters to highlight the context in which they appear and to put some perspective on their impact. A few comments on the papers are motivated for clarification, especially when new discoveries have been made since the time of their publication. We will also try to make an outlook to possible directions of further inquiries.

All results are of a theoretical nature, although some effort has been made to discuss the relevance for applications, mainly in the context of coupled optical waveguides. It can be verified that the parameter values used for the derived model equation are within ranges that are experimentally available, see Appendix A. But, as yet, we have found no reports in the literature of the fabrication of waveguide arrays with the nonlinear material present only inbetween the waveguides. As this is the geometry where nonlinear coupling can be of significant strength there is yet no experimental verification of the phenomena we have observed for the model with nonlinear coupling. However, based on the success of the cubic DNLS model with on-site nonlinearity to capture the phenomenology of arrays where also the waveguides are constructed from a nonlinear material, we can expect that the tight-binding approximation of our derivation should be an equally good model for arrays also with the former geometry. Further, though the strength of the parameters is in the range where many interesting effects of the nonlinear coupling occur, also their relative signs are of importance. The phase invariance of Eq. \( \text{(3.25)} \) lets us make some parameter transformations, e.g., the staggering transformation \( \Psi_m \mapsto (-1)^m \Psi_m \) which is equivalent to the change of parameters \( Q_2 \mapsto -Q_2 \) and \( Q_5 \mapsto -Q_5 \), and other transformations. Despite these transformations, the relative sign of \( Q_2 \) and \( Q_5 \) will always be the same as the Kerr index of the nonlinear material. Thus, the trick of working in the anomalous diffraction regime (Sec. 2.1.4) to effectively have different signs of \( Q_2 \) and \( Q_3 \) when the Kerr index
is positive cannot be used for the nonlinear coupling parameter.

The observation of compact excitations (Sec. 3.2.2) will thus truly require a material with negative Kerr index. Although this can be achieved for AlGaAs, one of the most commonly used dielectrics for waveguide arrays, the wavelength region where the nonlinearity is negative and of sufficient strength is connected to nonnegligible losses through absorption [120]. Other materials could therefore be needed to experimentally observe compatification in waveguide arrays. One should also consider that the compact solutions require an exact balance of the coupling parameters, expressed in the constraint of Eq. (3.44). While the fundamental DBs or vortices come in families, parameterized by the frequency or the norm, the compact solutions are isolated for fixed values of the coupling parameters. This means that they are not likely to survive as exact solutions for more accurate models beyond the tight-binding approximation. Note also that we cannot speak of strictly compact solutions even for the model of waveguide arrays, since the modes of the electric field in the waveguides are spatially exponentially localized.

Also, the change of direction of the norm current when the array is excited with plane waves is only possible with negative Kerr index. It is only in this case \((Q_2/Q_5 < 0)\) that the inversion of the current occurs over an interval of stable plane waves, see papers [III] and [V]. These phenomena are therefore maybe more easily observed in the context of Bose-Einstein condensates in a periodic potential (Sec. 2.2), where dilute gases corresponding to both signs of the nonlinear terms are available for experiments.

The issue of exchange of stability, and its connection to mobility of highly localized modes in a one-dimensional lattice (paper [I]), or lack thereof in a two-dimensional lattice (paper [V]), are obtained for both positive and negative values of the nonlinear coupling. To complement the results of paper [V] where the poor mobility is likely to be connected to the distance in phase space of the site-centred and bond-centred configurations, we can make some comparisons with the one-dimensional model [I]. As discussed in Sec. 1.2.6 we can heuristically view mobility of highly localized modes as a transformation between the two fundamental DBs, at least at low velocity and when the modes exchange their stability. At the instability threshold there is a depinning mode that is responsible for the transformation of one DB into the other. For fixed parameter values in the two-dimensional model there are points where the difference in Hamiltonian of the two stationary modes are zero, but still the bifurcation points where stability is changed are far apart from each other. Measuring the distance in norm between the site-centred and bond-centred configurations, we can see from Figs. 2 and 4 in paper [I] where the coupling is varied. Measuring instead the distance in the dynamical

\[ ^1 \text{Note first that after the initial parameter transformations in paper [I] we essentially have } Q_3 = K_3 = -0.5 < 0, \text{ while } Q_3 = 0.5 > 0 \text{ is used in paper [V] together with } Q_2 > 0 \text{ in both papers. Though it appears as if we have a focusing and defocusing case, respectively, the results are easily related to each other by making a staggering transformation, } \Psi_m \rightarrow (-1)^m \Psi_m, \text{ followed by a change of the direction of the time variable, } z \rightarrow -z. \text{ The effect is equivalent to changing the signs of } Q_3 \text{ and } Q_4 \text{ and noting that symmetric and anti-symmetric bond-centred solutions have changed meaning.} \]
Figure 4.1. Propagating excitations with very low velocity at a transparent point of Eq. (3.25). The parameters are $Q_2 = 0.2$, $Q_3 = -0.5$, $Q_4 = -0.1316$, $Q_5 = -0.1470$ and the norm is $N = 2.01464$. The calculations are made on a lattice with 51 sites and periodic boundary conditions. The site-centred solution has the Hamiltonian $H_1 = -2.61566$ and frequency $\Lambda_1 = -2.81196$ (with the sign convention used in Eq. (3.42), which is opposite to paper [1], while the symmetric bond-centred solution has frequency $\Lambda_2 = -2.81551$ and differs in Hamiltonian by $\Delta H = H_2 - H_1 = -1.6 \cdot 10^{-7}$. (a) Motion of the center of energy when the site-centred solution is perturbed by a phase gradient $(\exp(ikm))$. Note the time scale compared to the period of oscillation of the stationary solutions. For the solid line, $k = 10^{-4}$, and $H$ is increased by $7.0 \cdot 10^{-9}$ by the perturbation (which is less than the PN barrier, but we start very close to the solution with higher energy). For the dashed line, $k = 10^{-3}$, with an increase in $H$ of $7.8 \cdot 10^{-7}$. Note that the velocity for the slowest excitation is only $1.4 \cdot 10^{-4}$ sites/t.u.. (b) A snapshot of the slowest excitation at time $t = 10^3$. The tolerance for each component in the integration is $10^{-12}$, so the size of the tail is larger than the numerical accuracy.

In fact, as mentioned in paper [1], the distance between the bifurcation points can be zero, i.e., there are points where the stability of the site-centred and bond-centred solutions are exchanged at exactly the same time. Such points where termed transparent points in [145], where they were found for a model with saturable nonlinearity. At these points exact travelling solutions could be found without oscillations in the tail, but only for finite velocities. The existence of such points in the one-dimensional model with nonlinear coupling can be inferred from Fig. 4 in paper [1]. Since the site-centred and bond-centred solutions are simultaneously unstable in the left plot, with a stable intermediate solution, and simultaneously stable in the right plot, with an unstable intermediate solution, there must be a point inbetween where the bifurcation points coincide. At this point the site-centred and bond-centred solutions will have the same value of the Hamiltonian and the norm, but the frequency will not be exactly the same for the two modes, as we have confirmed in numerical calculations. Since also the region of existence of the intermediate solution, which connects the bifurcation points of the two fundamental DBs, degenerates into a point, all these stationary solutions must belong to a single family of solutions precisely at the transparent point. This means that the Peierls-Nabarro barrier truly is zero and a translationally invariant state must exist with a free parameter corresponding to the position parameter, the norm, we get $\Delta N/N \lesssim 0.05$. 
of its center relative to the lattice sites. As argued in [145] we may expect exact travelling solutions to bifurcate from such a point, where the translational state is the limit of zero velocity. These were also numerically obtained in [145], but due to resonances they can only have finite velocities. It could be interesting to further investigate the existence of exact travelling solutions also for the model with nonlinear coupling. Note that the condition for resonances with linear modes will be the same, and we should not expect to find exact travelling solutions with small velocity. This does not preclude that excitations can propagate with a low velocity at these points. Indeed, the numerical simulations presented in Fig. 4.1 show the center of energy of narrow excitations moving at a very small velocity at a transparent point of Eq. (3.25). These simulations alone cannot determine if the solutions are exact propagating solutions, but they appear to be essentially radiationless and the background is of the order $|\Psi_m|^2 \sim 10^{-13}$ (which, however, is above numerical accuracy). Note that the velocity is non-constant for the very slow excitation. At this very low velocity it is an effect of the, only to numerical precision vanishing, PN-barrier $|\Delta H| = 1.6 \cdot 10^{-7}$.

Just as for the compact solutions, the stationary phase twisted solutions come with a constraint, Eq. (3.45). But, with the phase difference between neighbouring sites, $\phi_{m+1}$, as an extra variable these solutions will still appear in families. It is a very interesting question whether solutions of this kind, with zero norm current, can be found in other models. In the model (3.25), it is the last term in the $Q_4$ part of the equation $(\Psi_m^* \Psi_{m+1}^2)$ that is needed for their existence. This term will in the Hamiltonian produce terms proportional to $\cos 2 \phi_{m+1}$, while the other coupling terms only give $\cos \phi_{m+1}$. The effect for the norm current is apparent from Eq. (3.38). Thus terms that couple strongly to the phase of neighbouring sites are needed. We should note that phase twisted solutions, with a non-zero energy flow, have previously been considered for KG lattices. These solutions were found by defining an effective action from the Hamiltonian of the dynamical equations (actually the Lagrangian is constructed), depending on the phases of the oscillations on each site. The extrema of this action then correspond to time-periodic solutions of the dynamical equations. The existence of solutions with non-trivial phase relations was proven in [14] based on the general existence proof from the anti-continuous limit. However, the studied solutions with non-trivial phases all represent an energy flow and have to form closed loops, i.e., they are really vortices [14, 49, 50]. Extremalizing the effective action gives constraints for the phase relations between neighbouring sites, expressed as the Euler-Lagrange equations in action-angle variables. When this procedure is applied to DNLS equations the relations of Eq. (3.36) are exactly reproduced. Compare, e.g., with the calculations in Appendix A in [102], but note that the Lagrange multiplier $\mu_n$ appearing in Eq. (A4) actually is identically zero for time-periodic solutions. In this context we may understand why there are likely no phase twisted stationary solutions with an open geometry in the KG lattices (nonlinear on-site potentials), since just as for the DNLS models we can expect that nonlinear interactions are

\[ An\ effective\ dynamics\ for\ the\ center\ of\ energy\ x_E\ would\ be\ \frac{d^2 x_E}{dt^2} \propto -\frac{\partial V_{PN}}{\partial x_E}, \]  where $V_{PN}$ is the PN potential. Thus, for a vanishing energy barrier, the velocity of the center of energy should be constant.
required. However, since phase twisted stationary modes exist in a DNLS model that is the rotating-wave approximation of the FPU lattices, Eq. (1.45), it could be interesting to see how these solutions translate into the full dynamics of FPU lattices. Note that the nonlinear interactions of these models are likely to give rise to terms with higher-order phase interactions, corresponding to \( \cos 2\phi_{m+1} \) and higher terms.

In paper IV we considered vortex solutions of the cubic DNLS equation, and especially ring-like configurations with or without the internal sites excited. Similar complexes of excitations carrying vorticity were also considered in [177] for continuum models with a periodic potential. The results coincide with the results of the tight-binding approximation in paper IV inasmuch as that there are no stable vortex rings with internal excited sites with vorticity \( S \geq 2 \). The excitations in [177] are only vortices oriented along square contours in the lattice and not diagonal configurations as in paper IV. We note also, that a large stable \( S = 2 \) vortex was computed in [176] for a continuum model with a periodic potential and the support of a parabolic trap. A further interesting development is that the effect of charge flipping of a vortex, which from the results of paper IV are connected to the existence of exact quasiperiodic excitations, has recently been observed in experiments on optically induced photonic lattices [25].

In connection to paper II and the investigation of the continuous nonlinear Schrödinger equation with nonlinear dispersion, we point out the important reference [125] that was overlooked. It addresses, among others, Eq. (3) in paper II with \( \gamma = \alpha = 0 \), and particularly proves the Vakhitov-Kolokolov (VK) stability criterion for this equation. It is also interesting to note that other forms of exotic solitons than the ones studied in paper II are possible. For Eq. (3.1) there are compactons in the limit of zero linear dispersion, and if we also consider solutions approaching a nonzero constant value at infinity there are dark (and anti-dark) compactons, compact kinks and dark, gray and anti-dark peaked solitons [156]. Further, in Sec. 3.1.2 we concluded that the phase is not allowed to vary in space for stationary localized solutions of Eq. (3.1) due to the form of Eq. (3.23) for \( C = 0 \). However, if the parameters \( \alpha_2 \) and \( \alpha_4 \) are of opposite signs this relation can be fulfilled for a particular amplitude without having \( \theta_c = 0 \) at that point. A consequence is that the phase can be allowed to vary for this particular amplitude, much in the same way as the slope can have discontinuities when the total dispersion vanishes. Thus it could be possible to have nonanalytic solitons where the phase has a discontinuity. The explicit form and stability properties of these are left for future investigations.

In conclusion, although we have described many interesting phenomena involving the nonlinear coupling of our model, a real challenge remains in investigating their wider applicability. If the mobility properties of narrow excitations are to be useful for multiport switching, or the transport properties of nonlinear plane waves for power steering, they must first be reproduced in experiments, and we must also investigate how they interact with each other and other excitations in the lattice. The same applies for the more exotic effects of stationary solutions if compactness and nontrivial phase relations of stationary modes are to be lifted from being mere mathematical curiosities. Still, also at this level they raise our
understanding of nonlinear dynamics, and who knows what discoveries they might inspire to? Since we have a fairly good understanding for the reason of their emergence, compactness being related to a vanishing coupling and nontrivial phases to a vanishing norm current, we have the tools to look for these phenomena also in other models. Thus, we can ultimately say that there is always more to be done.
Parameter estimates for optical waveguide arrays

A.1 One-dimensional array of slab waveguides

To demonstrate that the nonlinear coupling terms in Eq. (2.26) can be of significance in a realistic experimental setup we will calculate the coupling coefficients for a one-dimensional array of slab waveguides. The advantage of this configuration is the simplicity that makes it accessible to analytical treatment. Considering a single waveguide of width $2d$, as indicated in Fig. A.1, we make the ansatz $E(r, t) = E(y)e^{i(\beta z - \omega t)}$, where the mode $E(y)$ must satisfy the Helmholtz equation (2.3). Further, the mode will be confined if $k_0 n_i < \beta < k_0 n_e$, where $n_i$ and $n_e$ are the indices of refraction of the interior and exterior regions, respectively, and $k_0 = \sqrt{\mu_0 / \epsilon_0} \omega$ is the free space wave number. The mode with lowest propagation constant $\beta$ will be an even TE mode, with $E(y) = E(y)\hat{x}$ and a corresponding magnetic field $H(r, t) = H(y)e^{i(\beta z - \omega t)}$ given by Eq. (2.1),

$$\mathcal{H}_x = 0, \quad \mathcal{H}_y = \frac{\beta}{\mu \omega} E, \quad \mathcal{H}_z = i \frac{\partial E}{\mu \omega \partial y}.$$  \hfill (A.1)

Solving for the mode we arrive at \[ A \cos(kd)e^{\tilde{k}(y + d)} \quad y \leq -d, \]

$$E(y) = \begin{cases} 
A \cos(ky) & -d \leq y \leq d, \\
A \cos(kd)e^{-\tilde{k}(y - d)} & y \geq d, 
\end{cases} \hfill (A.2)$$

where $A$ is a constant. The wave numbers of the interior and exterior region, $k^2 = k_0^2 n_i^2 - \beta^2$ and $k^2 = \beta^2 - k_0^2 n_e^2$, can be combined to

$$(kd)^2 + (\tilde{k}d)^2 = (n_i^2 - n_e^2) k_0^2 d^2. \hfill (A.3)$$
From the boundary condition that the tangential components of the $E$ and $H$ fields, i.e., $E_x$ and $H_z$, are continuous at the interfaces ($y = \pm d$) another relation between the wave numbers follows,

$$\tilde{k}d = kd\tan(kd).$$

(A.4)

The intersection of Eq. (A.3) with Eq. (A.4) in a plot of $kd$ versus $\tilde{k}d$, will give the allowed wave numbers for propagating modes. For an odd TE mode, Eq. (A.4) is replaced with $\tilde{k}d = -kd\cot(kd)$, and it follows that we will have single-mode propagation if $0 < kd < \pi / 2$.

The constant $A$ is determined from the normalization, Eq. (2.8). Note that since the cross section of the waveguide is effectively one-dimensional the integration over $x$ is suppressed. $P_0$ will then be the power per unit length in the $x$ direction. Performing the integration with the mode (A.2) the result is

$$A^2 = \frac{2k\mu_0\omega P_0}{\beta(1 + kd)}.$$ 

(A.5)

Consider now an array of identical slab waveguides separated by a distance $s$, as shown in Fig. A.1 (a), such that if the mode $\mathcal{E}_m$ in waveguide $m$ is given by Eq. (A.2) the modes in the neighbouring waveguides are $\mathcal{E}_{m\pm1}(y) = \mathcal{E}_m(y \mp (s + 2d))$. We also assume that the interior region of the waveguides are constructed from a linear material, whereas the exterior region between the waveguides is nonlinear with Kerr index $n_2$. Since the mode (A.2) is exponentially decaying in the exterior region we will only integrate the coupling integrals, Eqs. (2.293a–c), over and between the neighbouring waveguides, while suppressing the integration over the infinite $x$ direction. The constant $Q_1$ is integrated over the neighbouring waveguides. The strength of the linear coupling $Q_2$ is calculated from the overlap.
of the mode with the mode in the nearest waveguide, i.e., the only non-zero part of the integration is over the region of the neighbouring waveguide. The coefficients related to the nonlinear terms in Eq. (2.26) should all be integrated over the region between the waveguides where the nonlinear material is present. Performing the integrations, and using Eqs. (A.3) and (A.4) to simplify the expressions, the results are

\[ Q_1 = -\frac{\varepsilon_0 \omega (n_i^2 - n_e^2)}{4kP_0} A^2 \cos^2(kd) e^{-2\tilde{k}(y-d)} dy \]

\[ = -\frac{\varepsilon_0 \omega (n_i^2 - n_e^2)}{4kP_0} A^2 \cos^2(kd) e^{-2\tilde{k}s} \left(1 - e^{-4\tilde{k}d}\right), \quad (A.6a) \]

\[ Q_2 = -\frac{\varepsilon_0 \omega (n_i^2 - n_e^2)}{4P_0} \int_{s+d}^{s+3d} (n_i^2 - n_e^2) A^2 \cos(kd) e^{-\tilde{k}(y-d)} \cos(k(y-s-d)) dy \]

\[ = -\frac{\tilde{k}}{2\mu_0 \omega P_0} A^2 \cos^2(kd) e^{-\tilde{k}s}, \quad (A.6b) \]

\[ Q_3 = -\frac{\varepsilon_0 \omega}{2P_0} \int_{d}^{s+d} n_e n_2 A^4 \cos^4(kd) e^{-2\tilde{k}(y-d)} dy \]

\[ = -\frac{\varepsilon_0 \omega n_e n_2}{8kP_0} A^4 \cos^4(kd) \left(1 - e^{-4\tilde{k}s}\right), \quad (A.6c) \]

\[ Q_4 = -\frac{\varepsilon_0 \omega}{4P_0} \int_{d}^{s+d} n_e n_2 A^4 \cos^4(kd) e^{-2\tilde{k}(y-d)} e^{-\tilde{k}(y-s-d)} dy \]

\[ = -\frac{\varepsilon_0 \omega n_e n_2}{4P_0} A^4 \cos^4(kd) e^{-2\tilde{k}s}, \quad (A.6d) \]

\[ Q_5 = -\frac{\varepsilon_0 \omega}{4P_0} \int_{d}^{s+d} n_e n_2 A^4 \cos^4(kd) e^{-3\tilde{k}(y-d)} e^{-\tilde{k}(y-s-d)} dy \]

\[ = -\frac{\varepsilon_0 \omega n_e n_2}{8\tilde{k}P_0} A^4 \cos^4(kd) e^{-\tilde{k}s} \left(1 - e^{-2\tilde{k}s}\right). \quad (A.6e) \]

The primary interest for our model is the relative strengths of the nonlinear couplings to the nonlinear self-interaction, which from the above expressions are given by

\[ \frac{Q_4}{Q_3} = \frac{\tilde{k}s}{\sinh 2\tilde{k}s}, \quad \frac{Q_5}{Q_3} = \frac{1}{2 \cosh \tilde{k}s}. \quad (A.7) \]

Hence, as can be seen in Fig. A.2, the nonlinear coupling terms are not negligible when the waveguide separation \( s \) is small or the penetration length \((\propto k^{-1})\) is large.
However, in an experimental setup we must also make sure that the input powers needed to operate the array are not too large. It turns out that the ratio of the linear coupling term to the on-site nonlinearity, i.e., \( |Q_2/2Q_3| \), is proportional to the power needed. The details can be found in paper [111] where the quotient appears as a rescaling of the amplitude. For the most interesting phenomena the rescaled amplitude is of the order 1, meaning that the constant of proportionality is of the order 1. Since \( Q_3 \propto n_2 \) a lower power input is needed for a material with large Kerr index. Using Eq. (A.5), together with \( \cos^2 kd = (kd)^2 + (\tilde{kd})^2 \) obtained from Eq. (A.4), we have from the expressions (A.6b) and (A.6c)

\[
\left| \frac{Q_2}{2Q_3} \right| = 1 \left( \frac{\mu_0 c_0 \omega^3 n_e n_2 P_0}{d^2 (kd)^2} \right) \frac{e^{-\tilde{kd} s}}{1 - e^{-4\tilde{kd} s}},
\]

(A.8)

From this expression we can make an order of magnitude estimate of the power. If the array is operated with a laser in the infra-red range with a wavelength \( \lambda \sim 1.5 \, \mu m \) we have a free space wave number \( k_0 \sim 5 \cdot 10^6 \, m^{-1} \) and a frequency \( \omega \sim 10^{15} \, \text{rad/s} \). If further the array is constructed from AlGaAs, with index of refraction \( n_e \sim 3.5 \) (and with \( n_i \sim n_e \)), reasonable sizes for the waveguides are in the tenth of micrometer regime, e.g., \( d \sim 5 \, \mu m \) and \( s \sim 10 \, \mu m \). We must also have \( kd \sim \tilde{kd} \sim 1 \) for single-mode propagation, which gives \( \tilde{kd} \sim 2 \) and \( \beta d \sim 25 \) \( (\beta \sim k_0 n_e \sim 5 \cdot 10^6 \, m^{-1}) \). The nonlinear properties of AlGaAs have been measured in [6]. For \( \lambda = 1.5 \, \mu m \) the result was \( n_2 = 1.9 \cdot 10^{-13} \, \text{cm}^2/\text{W} \), with the total index of refraction \( n = n_0 + \tilde{n}_2 I \). Since the intensity \( I = (\epsilon_0 \mu_0)^{-1} |E|^2 \) we convert this to \( \tilde{n}_2 = 5.0 \cdot 10^{-20} \, \text{m}^2/\text{V}^2 \) (cf Eq. (2.20)). Finally, with \( P_0 = 1 \, W/m \) we have that the power carried by the mode is \( |Q_2/2Q_3| P_0 \sim 2.2 \cdot 10^8 \, W/m \). If the array of waveguides is restricted also in the \( x \) direction, with a size of \( 10 \, \mu m \) the power is about 2 kW, which can be compared with the powers used in experimental setups with rectangular waveguides. In [144] the measured values of the coupling constants for an array of waveguides constructed from a nonlinear material, i.e., a slightly different configuration than considered here, is \( |Q_2/2Q_3| P_0 = 143 \, W \). We conclude that the powers needed to operate an array of waveguides with nonnegligible nonlinear coupling are accessible.
A.2 Two-dimensional array of square waveguides

For the two-dimensional array, Fig. A.1b, an analytical treatment is not as easy as for the one-dimensional array. The problem is that there is no known analytical solution for a rectangular dielectric waveguide. An approximate solution for modes not close to cut-off is given in [138], but in the exterior region it is only valid in the sections that share a boundary with the interior region, i.e., there are no expressions for the fields in the sections in the diagonal directions where the fields are assumed weak. From this solution we can nonetheless conclude that the relative sizes of the nonlinear coupling parameters to the on-site nonlinearity are about the same as for the array of slab waveguides, taking into account only the interaction in the region immediately inbetween two neighbouring waveguides. In the two-dimensional array there is also the possibility of coupling in the diagonal direction, between next-nearest neighbours. To estimate the strength of this linear coupling the approximate solution cannot be used. However, we can still make an order of magnitude estimate by taking expressions for the fields that will capture the essential behaviour in the separate regions, although this solution will not satisfy all the required boundary conditions and will exclude some field components (cf [138]). Requiring that the fields are oscillating in the interior region and exponentially decaying in the exterior region the dominating transverse field component of the electric field is taken as

\[
\mathcal{E}(x, y) = \begin{cases} 
A \cos(kx) \cos(ky) & -d \leq x, y \leq d, \\
A \cos(kd) \cos(ky) e^{-k(x-d)} & x \geq d, -d \leq y \leq d, \\
A \cos^2(kd) e^{-k(x-d)} e^{-\tilde{k}(y-d)} & x, y \geq d.
\end{cases} \tag{A.9}
\]

Since the waveguides are square, the wave numbers are the same for both directions in the lowest mode. The expressions are easily generalized to the regions not given in Eq. (A.9), but these will suffice for the present purpose. The mode is degenerate for a square waveguide, but the two orthogonal directions of polarization will ideally not interact, except under the presence of defects or a nonlinear material. In this case, since the modes have the same propagation constant \( \beta \) in an isotropic medium there is no need to distinguish between them. The assumption of single-mode propagation in Sec. 2.1.3 is therefore still valid. The same can be checked for the simplification in Sec. 2.1.2 of a preferred direction of polarization, provided that the material is isotropic. Thus the ratio of the linear direct coupling \( Q_2 \) to the linear diagonal coupling \( Q_D \) is

\[
\frac{Q_2}{Q_D} = \frac{\int_{-d}^d \int_{s+d}^{s+3d} \mathcal{E}(x, y) \mathcal{E}(x - s - 2d, y) \, dx \, dy}{\int_{s+d}^{s+3d} \int_{s+d}^{s+3d} \mathcal{E}(x, y) \mathcal{E}(x - s - 2d, y - s - 2d) \, dx \, dy} = \frac{\int_{-d}^d \cos^2(ky) \, dy}{\cos kd \int_{s+d}^{s+3d} e^{-k(y-d)} \cos(k(y - s - 2d)) \, dy} = \frac{e^{\tilde{k}y} [(kd)^2 + (\tilde{k}d)^2] \cos(kd)}{2(kd)^2 \sin(kd)}, \tag{A.10}
\]
where we have used Eq. (A.1), which is valid within the approximations of Eq. (A.9). An estimate of the size of this ratio, with $kd \sim \hat{kd} \sim 1$ and $s = 2d$, results in $Q_2/Q_D \sim 30$. Thus the nearest-neighbour coupling is at least an order of magnitude larger than the next-nearest-neighbour coupling for an array with square waveguides.
Bibliography


Bibliography


