Spectra and Dynamics of Excitations in Long-Range Correlated Structures

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Till min familj
Spectral and dynamical properties of electrons, phonons, electromagnetic waves, and nonlinear coherent excitations in one-dimensional modulated structures with long-range correlations are investigated from a theoretical point of view.

First a proof of singular continuous electron spectrum for the tight-binding Schrödinger equation with an on-site potential, which, in analogy with a random potential, has an absolutely continuous correlation measure, is given. The critical behavior of such a localization phenomenon manifests in anomalous diffusion for the time-evolution of electronic wave packets. Spectral characterization of elastic vibrations in aperiodically ordered diatomic chains in the harmonic approximation is achieved through a dynamical system induced by the trace maps of renormalized transfer matrices. These results suggest that the zero Lebesgue measure Cantor-set spectrum (without eigenvalues) of the Fibonacci model for a quasicrystal is generic for deterministic aperiodic superlattices, for which the modulations take values via substitution rules on finite sets, independent of the correlation measure.

Secondly, a method to synthesize and analyze discrete systems with prescribed long-range correlated disorder based on the conditional probability function of an additive Markov chain is effectively implemented. Complex gratings (artificial solids) that simultaneously display given characteristics of quasiperiodic crystals and amorphous solids on the Fraunhofer diffraction are designated. A mobility edge within second order perturbation theory of the tight-binding Schrödinger equation with a correlated disorder in the dichotomic potential realizes the success of the method in designing window filters with specific spectral components.

The phenomenon of self-localization in lattice dynamical systems is a subject of interest in various physical disciplines. Lattice solitons are studied using the discrete nonlinear Schrödinger equation with on-site potential, modeling coherent structures in, for example, photonic crystals. The instability-induced dynamics of the localized gap soliton is found to thermalize according to the Gibbsian equilibrium distribution, while the spontaneous formation of persisting intrinsic localized modes from the extended out-gap soliton reveals a phase transition of the solution.
Populärvetenskaplig sammanfattning

Vad karakterisera en kristall? Svar på denna till synes enkla fråga blir kanske att det är en anordning av atomer uppradade i periodiska mönstre. Så ordnade strukturer kan studeras genom att det uppträder så kallade Braggtoppar i röntgendiffraktionsmönstret. Om frågan gäller elektronlätenhet fördelnings, kanske svaret blir att denna är periodisk och grundar sig på elektronvägar som genomstränger hela kristallen. I och med att nya typer av ordnade system, så kallade kvasikristaller, upptäcks och framställs på artificiell väg blir svaren på dessa frågor mer intrikata.

En kristall behöver inte bestå av enheter upprepade periodiskt i rummet, och den klassiska metoden att karakterisera strukturer via röntgendiffraktionsmönstret kanske inte alls är den allena saliggörande. I denna avhandling visas att ett ordnat gitter vars röntgendiffraktionsmönster saknar inre struktur, dvs är av samma diffrusa typ som vad ett oordnat material uppvisar, fortfarande kan ha elektronerna utsträckta över hela strukturen. Detta implicerar att det inte finns något enkelt samband mellan diffriktionsmönstret från gittret och dess fysikaliska egenskaper såsom t ex lokaliserande av vågfunktioner. Man talar om lokaliserande när en vågfunktion är begränsad inom en del av materialet och inte utsträckt över hela dess längd, vilket är av betydelse när man vill avgöra huruvida ett material är en isolator, halvledare eller ledare. Det vittnar samtidigt om behovet av att söka efter andra karakteristika när man försöker beskriva skillnaden mellan ett ordnat och ett oordnat material, där den senare kategorin kan uppvisa lokalisering. Resultaten utgör en klassificering av det svåröverskäldliga området aperiodiska gitter i en dimension. Det leder till hypotesen att ideala kvasikristaller, genererade med bestämda regler, har kontinuerligt energispektrum av fraktal natur.

I reella material spelar korrelation en viktig roll. Vid icke-linjär återkoppling till gittret kan man erhålla intrinsiskt lokaliserade vågor, som i många avseenden beter sig som partiklar, solitoner, vilka har visat sig ha viktiga tillämpningar inom bl a optisk telekommunikation. Sådana vågors roll för lagring och transport av energi har undersökts i teoretiska modeller för optiska våglära och kristaller där ljuset har en förmåga att manipulera sig självt.
When I think back on the pleasant years spent in the Theoretical Physics group at Linköping University struggling with this thesis the first thought that comes to mind is my teaching of undergraduate students. A seemingly odd trick played by the subconscious mind that might be explained by my keen interest in the subject, but then again it has been my compulsive means of livelihood from time to time. However, this joyful activity has been rewarding in that I have been gaining a deeper understanding of certain areas in physics, such as electrodynamics, than I probably would have obtained otherwise. After all, there might be some truth to the saying “you learn as long as you have students”?

In this spirit I would like to express my sincere gratitude to Prof. Rolf Riklund, my supervisor, for being a great source of inspiration through his involvement in teaching as well as fundamental scientific research. I thank him for introducing me to the fascinating field of quasicrystals and aperiodic structures, which are subject to studies in this dissertation. The opportunity of working independently with projects of my own choosing, having background support and encouragement from Rolf, is very much appreciated. I can merely hope that some of my ignorant wonders amongst physical phenomena have contributed to the saying.

I have also been fortunate in having a co-advisor in Doc. Magnus Johansson. Besides a nice friendship he spreads enthusiasm for science and gladly shares his broad knowledge in nonlinear dynamics. Thank you, Magnus! Collaborations with Prof. Oleg Usatenko on correlated disorder and Prof. Alexander Kovalev on soliton dynamics, both from Kharkov in Ukraine, have been interesting experiences.

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My contribution to the science of elementary excitations in certain decorated lattices constitutes the heart of this dissertation – a collection of papers including:

**Paper I**  
L. Kroon, E. Lennholm, and R. Riklund  
*Localization–delocalization in aperiodic systems*  

**Paper II**  
L. Kroon and R. Riklund  
*Renormalization of aperiodic model lattices: spectral properties*  

**Paper III**  
L. Kroon and R. Riklund  
*Absence of localization in a model with correlation measure as a random lattice,*  

**Paper IV**  
O. V. Usatenko, S. S. Melnik, L. Kroon, M. Johansson, R. Riklund, and S. S. Apostolov  
*Spectral analysis and synthesis of 1D dichotomous long-range correlated systems: From diffraction gratings to quantum wires*  
Submitted

**Paper V**  
L. Kroon, M. M. Bogdan, A. S. Kovalev, and E. Yu. Malyuta  
*Bifurcation picture and stability of the gap and out-gap discrete solitons*  

**Paper VI**  
L. Kroon  
*The appearance of gap solitons in a nonlinear Schrödinger lattice*  
Manuscript

The following article is of related interest, but not included in the thesis:

**Paper VII**  
O. V. Usatenko, S. S. Melnyk, V. A. Yampol’skii, M. Johansson, L. Kroon, and R. Riklund  
*Three types of spectra in one-dimensional systems with random correlated binary potential,*  

This collection is preceded by a review of the studied field of wave (particle) phenomena in one-dimensional modulated structures with long-range correlations, which is intended to give a motivation and background to the scientific papers.

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Lars Kroon
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One of the miraculous aspects of Nature is its self-organizing ability of creating solid substances from different arrangements of atoms or groups of atoms at the microscopic level. An important goal for theoretical solid state physics is to develop an understanding of how the physical properties of a system are determined by its structure. A fundamental question to be answered in this context is the role of different types of correlations (order) among the atoms.

A limited aspect of this enormous task concerns the presence of localized or delocalized wavefunctions in quantum (or modes in classical) model systems exhibiting different types of correlations. This problem is closely related to the primary question of the propagation of particles or waves in inhomogeneous macroscopic structures. The dynamics of, e.g., an electronic wave packet in a structure that contains an arbitrary spatial distribution of scatterers is very difficult to predict. This is because of interference phenomena between parts of the wave packet successively scattered on the different scatterers, which depends on the strength and the spatial distribution of the scattering potential.

On one hand, if the potential distribution is completely regular, like for a periodic distribution, the interference between the scattered parts of the wave packet is coherent and long-range tunneling through the potential barriers can take place. A periodic solid, that is, a crystalline structure, is from a microscopic point of view built by repeating a unit cell, endowed with a basis of atoms, on a periodic lattice. The translational symmetry of a crystal implies that the single-electron wavefunctions are extended throughout the system according to Bloch’s theorem. The corresponding energy spectrum is absolutely continuous in that it consists of continuous bands for the infinite crystal. If the Fermi energy falls in the spectrum, the associated material can be an excellent conductor in which an electronic wave packet can show ballistic transport. One may note that even a perfect crystal can be an insulator (semiconductor), which happens if the bands
below the Fermi energy are completely filled at zero temperature. Let us just remind ourselves, that for a real crystal there will always be a certain amount of defects in the periodicity, like lattice vacancies or impurities. The presence of such a weak disorder can then be treated as a source of scattering for the Bloch states.

On the other hand, for a random potential distribution the interference between the partially scattered and transmitted waves can be destructive, something that may lead to localization of the wave packet in some region of space. The absence of periodicity makes Bloch’s theorem inapplicable, and the description of the system instead usually relies on statistical methods. The Anderson model [7] for site-diagonal disorder has been of fundamental importance for our understanding of the disordered structures, for example, the amorphous solids characterized by the absence of any long-range correlation. The fundamental character of the electronic states in the Anderson model depends strongly on the spatial dimension, which is in contrast to that of a periodic structure. It has been shown rigorously that in one dimension all states are exponentially localized for any amount of disorder [121, 125]. The electronic spectrum will then have a dense pure point character for the infinite system, and the associated material is an insulator. The most important results for higher dimensions follows from scaling theory of the dimensionless conductance or the localization length [2, 8, 49]. The conjecture is that in two-dimensional systems all states are localized at any level of disorder, while for sufficiently strong disorder in three dimensions a metal-insulator transition can occur if the Fermi energy is varied. In the latter case, for intermediate disorder, there are critical values of the energy, called mobility edges, dividing the bands into regions of extended states at the band center and regions of localized states at the band tails.

Figure 1.1. Displacive modulation, occupation modulation and composite structure from left to right are examples of incommensurate crystal phases. From Ref. [74].

In the beginning of the 1960s, structures which neither could be classified as periodic crystals nor amorphous materials were discovered [74]. In X-ray diffraction patterns of compounds like NaNO$_2$ and Na$_2$CO$_3$, relatively sharp satellite peaks were found indicating long-range order but incompatible with the positions of the main (Bragg) peaks. Materials with such properties were called incommensurate crystals, since they can be viewed as materials with two or more superimposed periodic structures with their periodicities incommensurate (irrational) with respect
to each other; see Fig. 1.1. In one-dimensional incommensurately modulated crystals the nature of the electronic eigenstates depends generically on the strength of the incommensurate (with respect to the lattice symmetry) modulation wave. For the famous self-dual Aubry-André model [12], the character of the electronic spectrum changes from absolutely continuous to pure point at the fixed point of duality, where the spectrum is singular continuous [15, 98]. The wavefunctions which belong to a singular continuous spectrum are usually called critical to emphasize that they are neither localized nor extended in the usual sense, but something in between. The criticality of localization is illustrated in Fig. 1.2 for two models.

![Figure 1.2. Electronic ground states for the tight-binding model with the quasiperiodic (a) Fibonacci and (b) period-doubling potentials using rigid boundary conditions.](image)

It is well known from group theory that translational symmetry imposes severe restrictions on the available invariant rotations of an object. In order to preserve periodicity the two-fold, three-fold, four-fold, and six-fold rotational symmetries are the only ones that are allowed [10]. In 1984, Shechtman et al. [146] published experimentally obtained electron diffraction patterns of a rapidly solidified Al-Mn alloy, which showed long-range orientational order having six axes of five-fold rotational symmetry. This symmetry group is known as the icosahedral group, which is not an allowed crystal point group. Soon afterwards, Levine and Steinhardt [102] showed theoretically, that materials which are built from a quasiperiodic repetition of different unit cells allow for rotational symmetries which are forbidden in translational invariant systems (cf. the planar Penrose lattice in Fig. 1.3). The term quasicrystal was introduced, and the icosahedral quasicrystals were shown to be possible. Quasicrystals are by definition solids whose atomic distributions have density functions which are quasiperiodic. A quasiperiodic function in turn is a superposition of a finite number of periodic functions with incommensurate periodicities. This means that the incommensurate crystals also are quasiperiodic structures. There are indeed some practical applications of quasicrystals. A certain type of steel (maraging) has a quasicrystalline structure from which it is armored and becomes strong and flexible, which is used in the production of suture needles. A quasicrystal is also used as a tough (ten times harder than stainless steal) and non-stick surface layer in frying pans (Cybernox®).

Besides the incommensurate crystals and quasicrystals, which occur in nature, there are also the artificial structures. By molecular beam epitaxy, one can build
superlattices by growing materials monolayer by monolayer on a substrate. In
the year 1985, Merlin et al. [117] built the first quasiperiodic superlattice with
two different layers of AlAs and GaAs ordered according to the famous Fibonacci
sequence, which can be viewed as an analogue to the Penrose lattice shown in
Fig. 1.3 These techniques have made it possible to perform experiments on both
deterministic aperiodic structures and amorphous multilayers. It has also been
proposed that aperiodic superlattices can provide promising alternatives to regular
photonic crystals for the realization of photonic devices, such as optical filters [38].

The Papers I–IV deal with localization properties of elementary excitations,
such as electrons, phonons and electromagnetic waves in one-dimensional modu-
lated lattices built from a finite number of entities. What is the nature of the
spectrum and to what extent does it depend on the diffraction measure of struc-
tural order? The possibility of using crystals as diffraction gratings was suggested
by von Laue in 1912. In the kinematic approach, assuming the atoms to be point
scatterers at integer lattice positions \( n \in \mathbb{Z} \), the radiation intensity \( I(k \equiv q_s - q_i) \)
of Fraunhofer diffraction of an incident plane wave with wave number \( q_i \) on the
sample is proportional to the Fourier transform

\[
\hat{C}(k) = \sum_r C(|r|) \exp(ikr). \tag{1.1}
\]

Here \( C(|r|) = \lim_{N \to \infty} \frac{1}{2N+1} \sum_{n=-N}^{N} \varepsilon(n)\varepsilon^*(n+r) \) is a two-point correlation
function of the scattering factor characteristics of the atoms \( \varepsilon(n) \) and \( r \) runs over all
the interatomic spacings. The wave number of the scattered monochromatic plane
wave is denoted by \( q_s \). The integrated intensity (cf. Fig. 1.4),

\[
\mu_I(k) = \int_{0}^{k} I(k')dk', \tag{1.2}
\]

introduces an intensity measure \( \mu_I(k) \), which can be used to classify the diffraction
spectra. This function attaches to any set of points in the coordinate space a
weight proportional to the diffracted intensity registered at \( k' \in (0,k) \). As any
monotone function, the measure \( \mu \) can be decomposed into a pure point (or atomic) part \( \mu_{pp} \), a singular continuous part \( \mu_{sc} \), and an absolutely continuous part \( \mu_{ac} \). The discrete part corresponds to the Bragg diffraction of periodic and quasiperiodic arrangements whose whole intensities are concentrated on \( \delta \) peaks. An absolutely continuous measure gives no weight to single points in the spectrum, whereas the weight of any interval is strictly positive. Such a measure is associated with the diffuse scattering present for (quasi-)random configurations. A singular continuous measure is an increasing continuous (Cantor-Lebesgue) function with a derivative equal to zero almost everywhere. In this view, the latter measure can be regarded as a characteristic of structural order in-between that of (quasi-)periodic and random distributions. Interestingly enough, there are deterministic aperiodic structures with their order “hidden” in the diffuse part of the Fourier intensity. One example is the Rudin-Shapiro model for which the correlation measure is a constant, and as such more homogeneous than that of a disordered lattice [128], see also Ref. [75] for experimental results.

The generation of structures with different correlations (order) among a finite set of entities and their associated dynamical systems are described in Chapter 2. The elucidation of the electronic properties of linear tight-binding Schrödinger models is outlined in Chapter 3. Chapter 4 is devoted to the treatment of phonons in the harmonic approximation of elastic vibrations, but also anharmonic phenomena in terms of discrete breathers – intrinsic localized modes are discussed.

An early account for intrinsic localization was given in a note by Landau in 1933 when describing the trapping of electrons in a crystal lattice [97]. The suggestion of polarization of the lattice due to a localized electron, which in turn would lower its energy, has led to the concept of the polaron, a quasiparticle viewed as the electron plus the induced localized lattice deformation. The polarization acts as a potential well, which through the dependence on the lattice distortion effectively depends on...
Figure 1.5. Arising of a discrete soliton through a modulational instability of a weakly nonlinear standing wave (phonon) with wave number \( k = \pi/2 \) in a discrete nonlinear Schrödinger equation with periodic on-site potential. Periodic boundary conditions are employed. Translational motion of the solitary wave appears at later times; see Paper VI.

itself. Such an intrinsic phenomenon abbreviated self-trapping or self-localization is now a widely recognized mechanism in condensed matter physics. The Holstein approximation \([67, 154]\) of the state with lowest energy for the electron-lattice interaction leads to an added cubic nonlinear diagonal term in the linear tight-binding model – a discrete nonlinear Schrödinger equation.

The continuous nonlinear Schrödinger equation, as the continuum limit of this nonintegrable discrete equation, has exact soliton solutions. The usual definition of a soliton is a localized solution to a nonlinear differential equation, representing a traveling wave of permanent shape, which can interact strongly with other solitons and retain its identity. The mathematical description of the properties of nonlinear waves is more subtle than the treatment of linear waves, which obey the principle of superposition. The term soliton was coined by Zabusky and Kruskal in 1965 to emphasize the particle-like properties observed in collisions of certain solitary waves \([150]\). The definition of a solitary wave as a localized wave that propagates in one space direction only, with almost undeformed shape, is in accordance with Ref. \([139]\) and inspired by the first documentation. This nice account is due to the engineer John Scott Russell who made the following observation in the Union Canal near Edinburgh in Scotland \([139]\):
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, . . .

A solitary wave, see Fig. 1.5 for a (stationary) discrete soliton, results from an exact balance between nonlinearity and dispersion, diffraction or diffusion. If this balance is not perfect it may lead to the formation of shock waves or the fragmentation of the initial condition. The focus in this thesis is upon lattices, and the inclusion of nonlinear terms to capture the prominent features of soliton-like excitations generally gives rise to nonintegrable systems, which allow for irregular and chaotic motion besides the spatially and temporally coherent structures. In Paper V and VI, the appearance of lattice solitons in a modulated discrete nonlinear Schrödinger equation is investigated. This equation, which is touched upon in Chapter 5 has shown success in the modeling of, for example, electromagnetic fields in waveguides, photonic crystals and Bose-Einstein condensates of ultracold atoms trapped in optical lattices.
CHAPTER 2

Symbolic dynamical systems

Long-range spatial or temporal correlations are of importance in many problems in modern physics, the theory of dynamical systems and also probability theory. The most natural approach to dynamical systems would be to accurately model a system taken from the vast reserve in Nature, but these systems are typically very complex in their structures. To better understand the role of correlations (order) among the atoms in materials, like quasicrystals, one-dimensional models are often generated by different ideal sequences. In this chapter some fundamentals of these symbolic sequences and their canonically associated dynamical systems are discussed along the lines in Ref. [128, 16]. The possibility to bring stochasticity into the problem using stationary additive Markov chains closes the mathematical approach. The discussion of the physical properties of the corresponding models is postponed to subsequent chapters.

2.1 Foundations

2.1.1 The symbolic language

We will consider a discrete finite set $\mathcal{A} = \{a_1, \ldots, a_d\}$ of elements. The elements are called letters and the set $\mathcal{A}$ an alphabet. The number $d \geq 2$ of letters in the alphabet is called the cardinality of the set, and is denoted by $\text{Card } \mathcal{A}$. Using the letters $a_i \in \mathcal{A}$, sequences of the type $(a_1a_2a_1a_2\cdots)$ can be constructed. A finite combination of letters like $v = a_1a_2a_1a_2$ is called a word, and the set of all such words over the alphabet $\mathcal{A}$ is denoted by $\mathcal{A}^*$. The product of two words $v$ and $\omega$, written as $v\omega$, is obtained by putting the word $\omega$ after the word $v$. This operation, called concatenation, is associative and has a unit element, the empty word, denoted by $\varepsilon$. The set $\mathcal{A}^*$ is thus endowed with
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the structure of a semi-group. Sometimes it is useful to extend this structure to a group by adding the formal inverses $a_i^{-1}$ of all the letters $a_i \in A$ as generators. Using the simplification rules $a_i a_i^{-1} = a_i^{-1} a_i = \varepsilon$ for the elements in the extended alphabet $\{a_1, \ldots, a_d, a_i^{-1}, \ldots, a_d^{-1}\}$ a group $\Gamma_A$ is obtained, which is called the free group generated by $A$. The concept of language is important when it comes to word combinatorics. If $v = v_1 \cdots v_n$ is a concatenation of $n$ words, $n$ is called the length of the word $v$. One defines the language $L_n(v)$ of length $n$ of a word $v$ as the set of all words of length $n$ in $A^\ast$ which occur in $v$.

A one-sided infinite sequence of elements from $A$ or a semi-infinite word is set to be an element $u = (u_n)_{n \in \mathbb{N}}$ in $A^\mathbb{N}$, where $\mathbb{N}$ denotes the natural numbers. The set $A^\mathbb{N}$ is a compact space when equipped with the product topology of the discrete topology on each copy of $A$, or equivalently with the distance $d(u, v) = d - \min\{n \in \mathbb{N} : u_n \neq v_n\}$. It is actually a Cantor set, i.e., a totally disconnected compact set without isolated points. Hence, two sequences are “close” to each other if their first symbols coincide.

2.1.2 Complexity and entropy

Is it possible to characterize the regularity of a given sequence $u$? A classical measure of disorder for sequences taking their values in a finite alphabet is the complexity function. It is a non-decreasing function $p_u(n)$ which with each positive integer $n$ associates $\text{Card} L_n(u)$, that is, the number of different words of length $n$ occurring in the sequence $u$. This function fulfills $1 \leq p_u(n) \leq d^n$. In fact, if there exists a positive integer $m$ such that the complexity function is bounded as $p_u(m) \leq m$, the sequence $u$ is eventually periodic. There is a natural notion of entropy associated with the complexity function. The topological entropy of a sequence $u$, defined by

$$H_{\text{top}}(u) = \lim_{n \to \infty} \frac{1}{n} \log_d p_u(n),$$

(2.1)

originates from topological dynamics [3]. There is a natural way of associating a dynamical system with a sequence. By defining the left-shift $S$ of $u$ by

$$Su \equiv S((u_n)_{n \in \mathbb{N}}) = (u_{n+1})_{n \in \mathbb{N}},$$

(2.2)

and taking the closure of the orbit (of $u$ under repeated application of the shift $S$) $\mathcal{O}(u) \equiv \{S^n u : n \in \mathbb{N}\}$, which is denoted by $X_u$, the pair $(X_u, S)$ is a topological dynamical system. Note that the shift $S$ is not one-to-one on $A^\mathbb{N}$, and that $X_u$ is finite if and only if $u$ is shift-periodic. A sequence $u$ is called shift-periodic if there exists a finite integer $m$ such that $S^m u = u$, which is the case for an ultimately periodic sequence. The topological entropy in (2.1) of the sequence $u$ is just the entropy of the dynamical system $(X_u, S)$. Clearly, the topological entropy satisfies $0 \leq H_{\text{top}}(u) \leq 1$, and it is zero for shift-periodic sequences. A sequence with entropy zero is said to be deterministic, while a sequence with entropy one is referred to as a normal sequence, which is sometimes taken as a signature of randomness.
2.1 Foundations

2.1.3 Substitution sequences

An efficient tool for generating sequences with low complexity functions, is by the use of substitutions. A substitution \( \sigma \) is an application from a finite alphabet \( \mathcal{A} \) into the set \( \mathcal{A}^* \). The substitution extends by concatenation to a morphism on \( \mathcal{A}^* \), that is, \( \sigma(v\omega) = \sigma(v)\sigma(\omega) \) and \( \sigma(\varepsilon) = \varepsilon \). It also extends in a natural way to a map over \( \mathcal{A}^\mathbb{N} \). A fixed point of the substitution \( \sigma \) is an infinite (substitution) sequence \( u \) obeying
\[
\sigma(u) = u.
\] (2.3)

If \( \sigma^m(u) \equiv \sigma(\sigma^{m-1}(u)) = u \) for some integer \( m \geq 1 \), the infinite sequence \( u \) is called a periodic point of \( \sigma \). The existence of at least one fixed point of a substitution \( \sigma \) is guaranteed, if there exists a letter (often called a seed) \( a_1 \in \mathcal{A} \) such that \( \sigma(a_1) \) begins with \( a_1 \), and that the length of the word \( \sigma^m(a_1) \) tends to infinity as \( m \to \infty \). The infinite sequence \( \sigma^\infty(a_1) \equiv \lim_{m \to \infty} \sigma^m(a_1) \) is then a fixed point of \( \sigma \), since it satisfies the relation (2.3). As an example, consider the Cantor substitution \( \tau \) defined over the alphabet \( \{a,b\} \) by \( \tau(a) = aba \) and \( \tau(b) = bbb \). The sequence of words \( (\tau^n(a))_{n \in \mathbb{N}} \) converges to a fixed point of \( \tau \), which is the Cantor sequence
\[
\tau^\infty(a) = ababababaababababaababababa\cdots.
\] (2.4)

A sequence \( u \) is called minimal (or uniformly recurrent), if every word occurring in \( u \) occurs in an infinite number of positions with bounded gaps. The iteration of \( \tau(b) = bbb \) in (2.4) gives no bounded gap so that the Cantor sequence is not minimal. That a sequence \( u \) is minimal is equivalent to the fact that the corresponding symbolic dynamical system \( (X_u, S) \) is minimal, which by definition means that for every point \( x \in X_u \) the orbit \( O(x) \) is dense in \( X_u \). Minimality of all the fixed points of a substitution \( \sigma \) is, however, guaranteed if \( \sigma \) is primitive. The primitivity means that for every \( a_i \in \mathcal{A} \), there is an integer \( m \) such that the word \( \sigma^m(a_i) \) contains all the letters in \( \mathcal{A} \). Hence, if the substitution \( \sigma \) is primitive, the corresponding substitution dynamical system denoted by \( (X_\sigma, S) \), which is generated by any of its periodic points, is the same for all the fixed points of \( \sigma \). This system is finite if and only if there is a periodic point for \( \sigma \) which also is shift-periodic. In this case, the substitution is also called shift-periodic.

2.1.4 Primitivity and ergodicity

The primitivity of a substitution \( \sigma \) on the alphabet \( \mathcal{A} \) with cardinality \( d \) can easily be expressed in terms of the substitution matrix (also called incidence matrix).

It is defined by the \( d \times d \) matrix \( M_\sigma \) whose entry of index \((i,j)\) is the number of occurrences of \( a_i \) in \( \sigma(a_j) \), where \( a_i, a_j \in \mathcal{A} \). Because of the identity \( M_\sigma^\infty = M_\sigma^n \), where the right-hand side stands for the \( n \)-th power of \( M_\sigma \), the application of this matrix over and over again gives information on the contents of letters in words of different lengths generated by the substitution. Indeed, the substitution \( \sigma \) is primitive if and only if there is an integer \( m \) such that \( M_\sigma^m \) has strictly positive entries only. When this holds true also the matrix is said to be primitive. For
the purpose of illustration, the substitution matrix for the Cantor substitution $\tau$ defined above reads

$$M_\tau = \begin{pmatrix} 2 & 0 \\ 1 & 3 \end{pmatrix}.$$  (2.5)

The matrix (2.5) is not primitive because $M_\tau^m$ always has one entry that is zero for every integer $m \geq 1$. The substitution matrix can also be used for calculating the weighted frequencies of words or the relative densities of the letters in a fixed point generated by a primitive substitution. A primitive matrix always admits a positive eigenvalue which dominates in modulus over the other eigenvalues. The coefficients of the eigenvector corresponding to the largest eigenvalue of the substitution matrix determine the relative densities of letters in the fixed point [128].

The main focus here is on primitive and not shift-periodic substitutions, which generate aperiodic fixed points having at most linearly growing complexities, that is, $p_u(n) \leq Cn$, for some constant $C$ and for all $n \in \mathbb{N}$. Even though the completely deterministic sequences have zero topological entropies, they can be characterized in terms of the spectral measures of their associated dynamical systems. A topological dynamical system always has a shift-invariant positive measure, that is, a measure $\mu$ invariant under the shift $S$. For a primitive substitution $\sigma$ this measure is unique, and the substitution dynamical system $(X_\sigma, S, \mu)$ is said to be uniquely ergodic. One may notice that the term ergodic stems from ergodic theory. The physical meaning of the celebrated ergodic theorem is that, under the relatively mild condition of ergodicity, the ensemble and “time” averages coincide.

### 2.2 Correlation measure

For an infinite sequence $u = (u_n)_{n \in \mathbb{N}}$ with values in a finite alphabet $\mathcal{A} \subset \mathbb{C}$, where $\mathbb{C}$ denotes the complex numbers, one can associate a family of positive measures on the one-dimensional torus $\mathbb{T}$, which can be considered as spectral types of the corresponding dynamical system $(X_u, S, \mu)$, equipped with a positive measure $\mu$.

Let us call a sequence $u$ regular, if the two-point correlation function defined by the sequence

$$C_u(m) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} u_n u^*_n + m,$$  (2.6)

exists for every $m \in \mathbb{N}$ (where the star denotes complex conjugation). If the definition of $C_u(m)$ in Eq. (2.6) is extended to the negative numbers through $C_u(-m) = C_u^*(m)$ the sequence $C_u = (C_u(m))_{m \in \mathbb{Z}}$ is positive definite. Then the Bochner-Herglotz theorem asserts that there is a positive measure $\mu_u$ on $\mathbb{T}$, such that the Fourier transform

$$\hat{\mu}_u(m) = \int_{\mathbb{T}} e^{i 2\pi mt} d\mu_u(t) = C_u(m),$$  (2.7)

for all $m \in \mathbb{Z}$. The measure $\mu_u$ is called the correlation measure of the sequence $u$, and it is unique when $u$ is regular. The correlation measure gives not only information about the averages of the sequence, but also about the so-called Fourier-Bohr
2.3 Deterministic aperiodic chains

spectrum defined by

$$S = \{ t \in T : \lim_{N \to \infty} \frac{1}{N} |U_N(t)| \neq 0 \},$$  \hspace{1cm} (2.8)

where $U_N(t)$ denotes the partial Fourier series

$$U_N(t) \equiv \sum_{n=0}^{N-1} u_n e^{-i2\pi nt}$$  \hspace{1cm} (2.9)

of the sequence $u$. It can be proven that for almost any sequence $u \in \{1, -1\}^\mathbb{N}$ the modulus of the partial Fourier series in Eq. (2.9) is bounded as

$$\sqrt{N} \leq \sup_{t \in [0,1)} |U_N(t)| \leq C \sqrt{N \log N},$$  \hspace{1cm} (2.10)

where $C$ is some constant. Indeed, there do exist a deterministic sequence, the Rudin-Shapiro sequence described in Section 2.3.3, such that the upper bound in (2.10) is sharpened to $(2 + \sqrt{2}) \sqrt{N}$. Its Fourier transform is a constant and its correlation measure is thereby identified as the Lebesgue measure. This is an example of a perfectly ordered sequence with an absolutely continuous correlation measure, like what is valid for an uncorrelated random sequence.

In order to put the Fourier intensity measure discussed in the introduction on a more clear mathematical ground, we return to the division of an arbitrary positive measure $\mu$. It can be divided into a pure point (discrete) part $\mu_{pp}$ and a continuous part, which in general is a sum of an absolutely continuous part $\mu_{ac}$ and a singular continuous part $\mu_{sc}$ according to the Lebesgue decomposition theorem. The absolute continuity of $\mu_{ac}$ means that for each set $T_a$ of zero Lebesgue measure $\mu_{ac}(T_a) = 0$, which implies the existence of a Lebesgue integrable function $m(t)$ such that $d\mu_{ac} = m(t) dt$. In the opposite direction, $\mu_{sc}$ is by definition singular if there exists a set $T_s$ such that its complement has zero Lebesgue measure and $\mu_{sc}(T_s) = 0$. The part $\mu_{sc}$ is a monotone continuous function (sometimes referred to as a devil’s staircase) with derivative equal to zero almost everywhere.

If a regular sequence has a continuous correlation measure $\mu_c$, that is, $\mu_c\{t\} = 0$ for all single points $t \in T$, the spectrum $S$ in (2.8) is empty. This is in contrast to a periodic sequence whose correlation measure is pure point. The correlation measure of a regular sequence can in principle consist of all three parts, and it is often used as an indicator of the complexity of sequences. Indeed, there are examples of correlation measures of each spectral type within the class of deterministic aperiodic sequences.

2.3 Deterministic aperiodic chains

This section contains a brief description of some deterministic aperiodic sequences, which here are obtained by the use of substitution rules. Some of these sequences allow for alternative generating procedures, such as finite automata, and the reader is referred to the dissertation for this approach. The selection of models is based on the fact, that their correlation measures are of different spectral types or that they are studied in the appended papers.
2.3.1 The Fibonacci model

In a simple model of rabbit breeding by Leonardo da Pisa (known as Fibonacci) in 1202, the following sequence of numbers occurred:

\[ \mathbb{F} = \{1, 1, 2, 3, 5, 8, 13, 21, \ldots, F_n, \ldots\} \quad (2.11) \]

Each of these so-called Fibonacci numbers \( F_n \) is the sum of its two predecessors, \( F_{n+1} = F_n + F_{n-1} \) (counting from the third number), which can be written as

\[ \begin{pmatrix} F_{n+1} \\ F_n \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} F_n \\ F_{n-1} \end{pmatrix}, \quad (2.12) \]

where the \( 2 \times 2 \) matrix is primitive. From a symbolic point of view, this matrix can be considered to be associated with a primitive substitution \( \sigma \) defined on the alphabet \( \mathcal{A} = \{a, b\} \) by the rule

\[ \sigma(a) = a \ b, \quad \sigma(b) = a. \quad (2.13) \]

In the original model of rabbit breeding, this means that an adult rabbit gives birth to a baby rabbit which grows up to an adult in every generation, and the infinite ordered population of rabbits is the fixed point

\[ \sigma^\infty(a) \equiv \lim_{n \to \infty} \sigma^n(a) = a \ b \ a \ b \ a \ b \ a \ b \ a \ b \ \cdots, \quad (2.14) \]

which is referred to as the Fibonacci sequence. The total number of letters in each word \( \sigma^n(a) \) (generation \( n \geq 1 \)) is obviously the Fibonacci number \( F_n \), where \( F_{-1} = 1 \) and \( F_0 = 1 \). The largest eigenvalue of the matrix in (2.12) is the golden mean \( \lambda_\tau = (1 + \sqrt{5})/2 = \lim_{n \to \infty} F_{n+1}/F_n \) (the other is \( \lambda_\tau^{-1} \)), with a corresponding eigenvector \((1, \lambda_\tau^{-1})^T\). Since the relative density of the letters in the fixed point is an irrational number the Fibonacci sequence cannot be periodic.

\[ \text{Figure 2.1. The intersection between a line with the slope } \lambda_\tau^{-1} \text{ (the inverse golden mean) and a two-dimensional integer grid generates the Fibonacci sequence.} \]
2.3 Deterministic aperiodic chains

It can be shown that the Fibonacci sequence is quasiperiodic (generated by two incommensurable frequencies), and its correlation measure is consequently pure point \[13\]. The complexity function is \( p_u(n) = n + 1 \) for all positive integers \( n \), which suggests that the Fibonacci sequence can be obtained by considering a line with the irrational slope \( \lambda_+ \) in a two-dimensional integer grid, counting the letter \( a \) whenever the line intersects a vertical and the letter \( b \) when it intersects a horizontal; see Figure 2.1. This model can also be considered to be a one-dimensional analogue to the two-dimensional quasiperiodic Penrose lattice \[57, 126\] and to the three-dimensional icosahedral quasicrystal \[102, 146\].

The Fibonacci model belongs to the class of substitutions which are invertible. A substitution \( \sigma \) can also be extended to the free group \( \Gamma_A \) by defining \( \sigma(a_i^{-1}) = (\sigma(a_i))^{-1} \) for the inverses \( a_i^{-1} \) of the letters \( a_i \in A \). It is said to be invertible, if there exists a map \( \sigma^{-1} \) over all of \( \Gamma_A \) such that \( \sigma^{-1} \sigma = \sigma \sigma^{-1} = \varepsilon \), where \( \varepsilon \) is the identity. It is easy to show that the inverse of the substitution (2.13) is given by

\[
\sigma^{-1}(a) = b, \quad \sigma^{-1}(b) = b^{-1}a,
\]

which may be called the inverted Fibonacci substitution.

2.3.2 The Thue-Morse model

A famous example of an infinite sequence of symbols from an alphabet \( A = \{a, b\} \) that does not contain any cubes, that is, three identical words in succession, is

\[
u = a b b a b a a b b a a b a a b b a b a a b b a b b a \ldots .
\]

This sequence was constructed by Thue in 1906 \[151, 152\] for that purpose, and it was rediscovered in 1921 by Morse \[120\] in the context of coding geodesics on surfaces. The sequence of symbols (2.16) can be obtained by an obvious iteration of the substitution

\[
\sigma(a) = ab, \quad \sigma(b) = ba,
\]

and the fixed point \( u = \sigma^\infty(a) \) is called the Thue-Morse sequence. The corresponding substitution matrix

\[
M_\sigma = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}
\]

has the same form as that of a periodic substitution rule, but the Thue-Morse sequence is neither periodic nor quasiperiodic. However, there are words in the sequence that read the same backwards as they do forwards, such as the words \( abba \) and \( baab \), which are called palindromes. The Thue-Morse sequence is an example of a palindromic sequence, which by definition means that it contains arbitrarily long palindromes. Indeed, the word \( \sigma^n(a) = \sigma^{n-1}(a)\sigma^{n-1}(b) \) is easily seen to be symmetric (antisymmetric) with respect to the middle point for every even (odd) integer \( n \).

The complexity function of the Thue-Morse sequence has a less simple expression, but it fulfills \( p_u(n) < 4n \) for all positive integers \( n \). If the letters in
the alphabet are coded with the numbers \(\{1, -1\}\), the correlation measure of the Thue-Morse sequence \(u \in \{1, -1\}^\mathbb{N}\) is purely singular continuous \([110]\). Actually, the convergence of the correlation function \((2.6)\) can be understood as a consequence of unique ergodicity of the associated dynamical system \((X_u, S)\). That is, the \(m\)th Fourier coefficient \(\hat{\mu}_u(m)\) of the correlation measure, which here is the Riesz product \(\prod_{n \geq 0} (1 - \cos 2^n t) \) \([128]\), equals the correlation function \(C_u(m)\), which is non-zero for infinitely many \(m \geq 0\).

### 2.3.3 The Rudin-Shapiro model

The question of whether there existed a sequence \(u \in \{1, -1\}^\mathbb{N}\) for which the modulus of its partial Fourier series in Eq. \((2.9)\) is bounded as \(\sqrt{N} \leq |U_N| \leq C\sqrt{N}\) for some constant \(C\) and any positive integer \(N\) was linked to several problems in harmonic analysis. One example of a sequence meeting this requirement is the \textit{Rudin-Shapiro sequence} \([136, 145]\), which can be obtained from the recursion

\[
\begin{align*}
    u_0 &= 1, \\
    u_{2n} &= u_n, \\
    u_{2n+1} &= (-1)^n u_n.
\end{align*}
\]

This sequence is obviously deterministic, its complexity function is \(p_u(n) = 8n - 8\) for all \(n \geq 8\), and one would expect its behavior to be very far from that of a random sequence. In particular, positive correlations should be expected, like for the Thue-Morse sequence. However, the correlation measure of the Rudin-Shapiro sequence is the Lebesgue measure for which the Fourier transform is the constant \(\hat{\mu}_u(0)\) \([128]\), so that the correlation function \(C_u(m) = 0\) for all \(m \geq 1\). This is thus a result pointing in the opposite direction.

Recoding the numbers \(\{1, -1\}\) building the Rudin-Shapiro sequence by the letters from the alphabet \(\mathcal{A} = \{a, b\}\), the corresponding symbolic sequence \(u\) reads

\[
u = a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a b a b a a
It can also be obtained from a substitution $\sigma$ defined on the binary alphabet $\mathcal{A} = \{a, b\}$, where the rule takes the form
\[
\sigma(a) = ab, \quad \sigma(b) = aa,
\]
and the fixed point
\[
\sigma^\infty(a) = a b a a a b a b a a a b a a a b a a a b a b a b \cdots
\]
is called the period-doubling sequence. It belongs to a class of sequences which are denoted limit-periodic sequences \[90, 91\], which by definition means that its spectral measure consists of Bragg peaks at values obtained as rational multiples of a single frequency. Hence, the correlation measure of the period-doubling sequence is pure point, like what is valid for periodic and quasiperiodic sequences.

### 2.4 Additive Markov chains

For a binary random sequence of symbols $\varepsilon(n) \in \{\varepsilon_0, \varepsilon_1\}$, where $n \in \mathbb{Z}$, the $N$-step Markov chain is introduced via the conditional probability $P(\varepsilon(n) \mid T_{N,n})$, which is the probability for the definite symbol $\varepsilon_m$ ($m \in \{0, 1\}$) to occur after the sequence of symbols $T_{N,n} \equiv (\varepsilon(n - N), \varepsilon(n - N + 1), \cdots, \varepsilon(n - 1))$. The additive Markov chain is then defined by the probability function
\[
P(\varepsilon(n) = \varepsilon_1 \mid T_{N,n}) = p_1 + \sum_{r=1}^{N} F(r) \left( \frac{\varepsilon(n - r) - \langle \varepsilon(n) \rangle}{\varepsilon_1 - \varepsilon_0} \right),
\]
where $p_1$ ($p_0 = 1 - p_1$) is the relative part of symbols $\varepsilon_1$ ($\varepsilon_0$) among the set of symbols in the entire sequence. Due to ergodicity, the average along the sequence
\[
\langle \varepsilon(n) \rangle \equiv \lim_{M \to \infty} \frac{1}{2M + 1} \sum_{n=-M}^{M} \varepsilon(n) = \varepsilon_0 p_0 + \varepsilon_1 p_1
\]
is equivalent to the ensemble average of realizations of the stationary Markov chain with $p_0 + p_1 = 1$. The quantity $F(r)$ is referred to as the memory function \[155\], which describes the effect of correlations between the nth symbol $\varepsilon(n)$ and the previous string of symbols $\varepsilon(n - r)$ for $r = 1, \ldots, N$. The conditional probability depends on the parameters $p_0$, $p_1$ and the length $N$ of the “memory” for the step-like memory function, but not on the arrangement within the $N$-word.

The interest in the memory function resides in its connection to a correlation function. The two-point correlation function (as used in Paper IV differ slightly from the form (2.6)) of a real-valued random sequence $\varepsilon(n)$ is here defined as
\[
C(r) = \langle \varepsilon(n)\varepsilon(n + r) \rangle - \langle \varepsilon(n) \rangle^2.
\]
This is an even function, $C(-r) = C(r)$, with the variance $C(0) = (\varepsilon_1 - \varepsilon_0)^2 p_0 p_1$. There is a single-valued relation between the memory function $F(r)$ and the normalized correlation function $K(r) = C(r)/C(0)$ \[116, 117\], which reads
\[
K(r) = \sum_{r'=1}^{N} F(r') K(r - r'), \quad r \geq 1.
\]
This equation allows for the calculation of the memory function $F(r)$ from a prescribed correlator $K(r)$ and the construction of the Markov chain effectively using the conditional probability $0 \leq P(\cdot \mid \cdot) \leq 1$ in Eq. (2.24). Apart from very specific choices of correlations no general results on the existence of solutions to Eq. (2.27) in the limit $N \to \infty$ are known to the present author [71]. For not too large memory functions $F(r)$ numerical matrix inversion of the equation

$$
\begin{pmatrix}
K(1) \\
K(2) \\
\vdots \\
K(N)
\end{pmatrix} = 
\begin{pmatrix}
K(0) & K(1) & \cdots & K(N-1) \\
K(1) & K(0) & \cdots & \vdots \\
\vdots & \vdots & \ddots & K(1) \\
K(N-1) & \cdots & K(1) & K(0)
\end{pmatrix}
\begin{pmatrix}
F(1) \\
F(2) \\
\vdots \\
F(N)
\end{pmatrix}
$$

(2.28)

works rather well for many choices of the correlator $K(r)$. One may notice that the function $F(r)$ is defined for $r \geq 1$, but analytical continuation as $F(-r) = F(r)$ to negative values of $r$ seems reasonable with some freedom of choice for $F(0)$. In the other direction, the correlation function can be calculated for a given memory.

In Paper IV, the possibility of using this method to merge discrete systems with different measures or order, expressed via their correlation functions in real space or in Fourier space, together into complex compounds is addressed (cf. the intensity measure of the diffraction patterns in Fig. 1.4, which are related to the Fourier transform of the correlation function). In order to apply the method to compositions in Fourier space, an inverse transform of the complex into real space should be performed in the first step. In view of characteristic functions, it suffices however to calculate the Fourier transform of a composed correlation function $C(r)$, presented in $k$-space via

$$
\hat{C}(k) = \sum_i \chi_{[k_1, k_2]}(k) \hat{C}_i(k),
$$

(2.29)

where the characteristic function $\chi_{[k_1, k_2]}(k)$ is equal to 1 if $k \in [k_1, k_2]$ and zero otherwise. Straightforward inverse transformation yields (Paper VII)

$$
C(r) = \sum_i \left\{ \frac{k_2 - k_1}{\pi} C_i(r) + \sum_{r' = 1}^{\infty} \sin \frac{k_2 r' - k_1 r'}{\pi r'} [C_i(r + r') + C_i(r - r')] \right\},
$$

(2.30)

where $\{C_i\}$ are correlation functions for the different discrete systems $\{i\}$. In the case when $\hat{C}_i = 1$, the expression (2.30) reduces to the only term

$$
C_\chi(r) = \begin{cases} 
\frac{\sin k_2 r - \sin k_1 r}{k_2 - k_1} & r \neq 0, \\
\frac{\pi r}{k_2 - k_1} & r = 0,
\end{cases}
$$

(2.31)

which is just the Fourier transform $\frac{1}{\pi} \int_0^\pi \chi_{[k_1, k_2]}(k) \cos(kr) dk$ of the characteristic function $\chi$. 

Symbolic dynamical systems
The purpose of this chapter is to give an overview of the treatment of simple tight-binding models for the electronic structure in one-dimensional aperiodic crystals (superlattices), for which the usual band theory of periodic solids is ruled out due to the absence of a finite Brillouin zone, and purely stochastic methods do not apply either. The discussion involves some spectral theory of discrete Schrödinger operators, its relation to the dynamical localization properties, and the diffusion processes of excitations in the systems. The Thue-Morse chain is considered as a prototype model in order to show how the formalism applies. Electronic properties of some of these models and related ones are also studied in Refs. [47, 77, 68].

3.1 Tight-binding models

The basic starting point is the time-independent Schrödinger equation

$$\mathcal{H} |\Psi\rangle = E |\Psi\rangle.$$  \hfill (3.1)

We consider a one-dimensional lattice where each atom contributes with only one orbital, and where the spin-orbit coupling is ignored. In determining the spectrum, that is, the allowed values of the energy $E$, for a single electron in the discrete lattice, the Hamiltonian

$$\mathcal{H} = \sum_n V_n |n\rangle \langle n| + \sum_{n\neq m} t_{n,m} |n\rangle \langle m|,$$  \hfill (3.2)

is widely used. This is the tight-binding approximation [10] for which it is assumed that the atomic orbital $|n\rangle$ centered around site $n$ overlaps weakly with the atomic orbitals at the other lattice sites. The hopping (overlap) matrix element between
the atoms at site \( n \) and \( m \) is denoted by \( t_{n,m} \), and \( V_n \) is the on-site potential. Here, the analysis is restricted to nearest-neighbor interaction, that is, \( t_{n,m} = 0 \) when \( |n - m| \neq 1 \). The total state vector of the electron is also expanded in the atomic orbitals as

\[
|\Psi\rangle = \sum_n \psi_n |n\rangle.
\] (3.3)

Such an expansion is always possible for a periodic lattice, since the states can be chosen as the Wannier orbitals \([10]\). It has been proven that exponentially localized (generalized) Wannier functions indeed exist for a rather wide class of nonperiodic potentials \([122]\), which may justify the expansion (3.3) in studying aperiodic lattices. Multiplying the Schrödinger equation (3.2) with the bra-vector \( \langle n \mid \) for the state (3.3) yields the system of equations

\[
V_n \psi_n + t_{n,n+1} \psi_{n+1} + t_{n,n-1} \psi_{n-1} = E \psi_n,
\] (3.4)

for the wavefunction coefficients \( (\psi_n)_{n \in \mathbb{Z}} \). Inferring the vectors \( \Psi_n = (\psi_{n+1}, \psi_n)^T \), the relation (3.4) is conveniently rewritten as the difference equation

\[
\Psi_n = \tilde{T}_n \Psi_{n-1}, \quad \tilde{T}_n \equiv \begin{pmatrix}
(E-V_n) & -t_{n,n+1} \\
t_{n,n+1} & 1
\end{pmatrix}.
\] (3.5)

In Paper I the on-site (diagonal) model is studied, which is achieved by choosing all the hopping matrix elements equal to a constant and the modulation is introduced in the site energies. In this case the transfer matrices \( \tilde{T}_n \) have determinants equal to one, and they belong to the group \( \text{SL}(2, \mathbb{R}) \), consisting of real, unimodular \( 2 \times 2 \) matrices. If instead the hopping matrix elements are modulated and the on-site energies are constant the transfer (off-diagonal) model is obtained. From a physical point of view, one expects that the hopping matrix elements, coupling two neighboring atoms in the lattice, are determined by their electronic structure which, in turn, define a certain distribution of on-site energies along the chain. In this respect, variations of both the diagonal and the off-diagonal elements give more realistic mixed models. For mixed models not all of the transfer matrices are unimodular, which makes the study of the spectral properties of the systems more difficult. In Paper II mixed models are studied analytically, where the hopping matrix elements are modulated in correlation with binary distributions of on-site energies. By the use of renormalization procedures, these mixed models are transformed to on-site models of renormalized lattices described by unimodular transfer matrices. This is also of interest when studying elastic vibrations in harmonic lattices with aperiodic modulations of masses; see Section 4.1. If all the hopping matrix elements are normalized to \(-1\) in Eq. (3.4), the system is equivalent to the discrete time-independent Schrödinger equation in units such that \( \hbar^2/(2m) = 1 \) and with energy \( E + 2 \).

Throughout this chapter, all the hopping matrix elements \( t_{n,n+1} \) are normalized to unity. For this on-site model the potential \( V_n = v(\omega_n) \) is generated from a fixed point \( u = (u_n)_{n \in \mathbb{N}} \) of a primitive substitution \( \sigma \) defined on a finite alphabet \( \mathcal{A} \) by the use of an injective map \( v \), that is, a projection from \( \mathcal{A} \) to the set of real
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The potential needs to be extended to the negative numbers, \( n < 0 \), which can be accomplished by taking elements from the alphabet \( \mathcal{A} \), constructing an infinite sequence \( \omega = (\omega_n)_{n \in \mathbb{Z}} \) such that \( \omega_n = u_n \) for \( n \geq 0 \). The corresponding Hamiltonian is denoted by \( H_\omega \) to emphasize that the on-site potential depends on the element \( \omega \). The associated substitution dynamical system, denoted by \((\Omega_\sigma, S)\), is constructed by taking \( \Omega_\sigma \) as the set of accumulation points of \( \{S^n\omega : n \in \mathbb{N}\} \) under the left-shift \( S \) defined in (2.2) (extended to \( n \in \mathbb{Z} \)). This procedure makes \((\Omega_\sigma, S)\) minimal and uniquely ergodic \([128, 65]\), which is a natural extension of sequences and their associated substitution dynamical systems from \( \mathcal{A}^\mathbb{N} \) to \( \mathcal{A}^\mathbb{Z} \).

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The characterization of the electronic wavefunctions requires an investigation of the spectrum of the (self-adjoint) Hamiltonian \( H_\omega \), which by definition is the complement of the set of values \( E \) such that the resolvent \((H_\omega - E)^{-1}\) is a bounded operator. This is a closed set, which is denoted by \( \Sigma(H_\omega) \). The spectrum contains all of the eigenvalues of \( H_\omega \), that is, all energies \( E \) for which the equation

\[
H_\omega \psi = E \psi
\]

admits a normalized solution \( \psi = (\psi_n)_{n \in \mathbb{Z}} \) in the space \( l^2(\mathbb{Z}) \). The closure of the set of eigenvalues is called the pure point part of the spectrum, denoted by \( \Sigma_{pp}(H_\omega) \). The solutions to equation that are not square normalizable belong to the continuous spectrum, which further can be divided into a disjoint union of the absolutely continuous part \( \Sigma_{ac}(H_\omega) \) and the singular continuous part \( \Sigma_{sc}(H_\omega) \) according to the Lebesgue decomposition of the spectral measure. The absolutely continuous part is a closed set with non-empty interior, while the singular continuous part is a bit harder to capture in words (cf. the decomposition of a positive measure mentioned in the introduction and discussed in Section 2.2). The wavefunctions which belong to the absolutely continuous part are called extended, while those that belong to the singular continuous part of the spectrum are generally more exotic in nature, and are often denoted as critical due to large scale fluctuations in their charge distributions. However, the two latter types of wavefunctions are both non-normalizable (generalized eigenfunctions) in contrast to the localized eigenstates that are associated to the pure point part of the spectrum.

Let us return to the transfer matrix formulation of Eq. (3.6), where the corresponding matrix now is denoted by \( T \). Since the on-site potentials \( V_n = v(\omega_n) \) are generated by a substitution \( \sigma \) defined on an alphabet \( \mathcal{A} \), it is natural to define the map

\[
T(a_i) = \begin{pmatrix} (E - v(a_i)) & -1 \\ 1 & 0 \end{pmatrix}
\]

for every \( a_i \in \mathcal{A} \). This unimodular matrix is, with a slight abuse of notation, extended to operate also on an arbitrary word \( (a_1 \cdots a_{n-1} a_n) \in \mathcal{A}^* \) according to

\[
T(a_1 \cdots a_{n-1} a_n) \equiv T(a_n) T(a_{n-1}) \cdots T(a_1).
\]
Note that the order between the transfer matrices operating on each letter $a_i \in A$ is reversed with respect to the order of the letters in the word, which is consistent with the iteration of the difference equation (3.5). Now it is possible to combine the map (3.8) with the substitution $\sigma$ defined on the alphabet $A$ via

$$\sigma^m |T(a_i)| \equiv T^{(m)}(a_i) \equiv T[\sigma^m(a_i)] \quad (3.9)$$

under $m$ repeated applications of the substitution $\sigma$ to an arbitrary letter $a_i \in A$ (or to words in $A^*$ for that matter). Hence, each element $\omega$ in the sequence $\omega$ is replaced by the corresponding transfer matrix $T$ in the string $T(\omega)$, and this formalism also incorporates the application of the left-shift $S^m \omega$. Notice, however, that Eq. (3.9) is not invariant under finite shifts, since it generally gives rise to new substitution rules.

Given an initial vector $\Psi_0$, a vector $\Psi_n$ for arbitrary $n$ in the difference equation (3.5) can be found as $\Psi_n = R_n \Psi_0$, where $R_n$ is the total transfer matrix defined by

$$R_n = \begin{cases} T_n T_{n-1} \cdots T_1, & n \geq 1, \\ I, & n = 0, \\ T_{n+1}^{-1} T_n^{-1} \cdots T_0^{-1}, & n \leq -1, \end{cases} \quad (3.10)$$

where $I$ is the unit matrix. It turns out to be very useful to measure the rate of exponential growth of the solutions to the difference equation by the expressions

$$\Lambda_{\omega}^\pm (E) = \lim_{n \to \pm \infty} \frac{1}{n} \ln \| R_n(E) \|, \quad (3.11)$$

where $\| \cdot \|$ is the matrix norm, that is, the supremum over $\| \Psi_n \| = \| R_n \Psi_0 \|$ for some (linearly independent) initial vectors $\Psi_0$ with unit norm. When the limits in (3.11) exist and are equal, this number is called the Lyapunov exponent, denoted by $\Lambda_{\omega}(E)$. In the case of a positive Lyapunov exponent, one has a complete understanding of the asymptotics of the solutions at infinity, see for example \[99\] and references therein. In particular, if $\Lambda_{\omega}(E) > 0$ everywhere there can be no absolutely continuous part of the spectrum, and the localization length $\xi$ of the electron is bounded from below by the relation $\xi(E) \geq 1/\Lambda_{\omega}(E)$ \[36\], with equality for the Anderson model \[103\].

It has been proven that $\Lambda_{\omega}(E)$ exists for all $\omega \in \Omega_\sigma$ \[64\]. Moreover, the absence of an absolutely continuous part $\Sigma_{ac}$ of the spectrum has been established first by Hof et al. \[65\], and in general on a set of full measure by Last and Simon \[99\]. In 2002, Lenz \[101\] provided the hitherto most general result for the spectral character by showing that the spectrum is

$$\Sigma(H_\omega) = \{ E \in \mathbb{R} : \Lambda_{\omega}(E) = 0 \} \quad (3.12)$$

for all (aperiodic) $\omega \in \Omega_\sigma$. Since this set has Lebesgue measure zero \[65\], it follows that the spectrum $\Sigma$ is a Cantor set of zero Lebesgue measure. A general Cantor set is a closed, uncountable set with no isolated points (all points are limit points) and whose complement is everywhere dense. One may note that a general Cantor set is not necessarily of zero measure. However, the absence of isolated points of a
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Cantor set does not imply the absence of eigenvalues in the spectrum, since there can still be solutions decaying to zero at infinity. So the spectrum can be written

$$\Sigma(\mathcal{H}_\omega) = \Sigma_{sc} \cup \Sigma_{pp}(\mathcal{H}_\omega),$$  \hspace{1cm} (3.13)

which holds for a set of full measure. To the best of the present author’s knowledge there is no general method for proving the absence of the pure point part of the spectrum on all of $\Omega_\sigma$. The absence of localization in deterministic aperiodic models, that is, for some fixed $\omega \in \Omega_\sigma$ determined by certain (primitive) substitution rules, seems to be the generic behavior. The strong result in 5.12 suggests that if one member $\omega$ of the family $\Omega_\sigma$ is difficult to study, it might well be that another one is easier. This simple but fruitful idea is made use of in Paper III.

In order to exclude the presence of point spectrum for a given model, one must provide the knowledge that, for every energy $E$ in the spectrum, no solution of the Schrödinger equation tends to zero at infinity. A convenient tool for doing that is to study the dynamical system imposed by the relation (3.9) for a specific substitution rule. This method was applied in the pioneering studies of the Fibonacci model already in 1983 [89,124], one year before the actual discovery of quasicrystals [146]. This method is borrowed and generalized from that of periodic systems. For a periodic approximant of $\mathcal{H}_\omega$ having a unit cell with $n$ sites, the spectrum $\Sigma$ consists of all energies $E$ for which the corresponding wavefunctions $(\psi_n)$ satisfy the Bloch condition (Floquet theorem) $\psi_{j+n} = \exp(ikn)\psi_j$. Using the unimodularity of the corresponding transfer matrices in (3.10), the relation $\text{tr} R_n = 2\cos kn$ is obtained, where tr denotes the trace of the matrix $R_n$. The energy spectrum can then be written

$$\Sigma(\mathcal{H}_\omega(n)) = \{E \in \mathbb{R} : |\text{tr} R_n| \leq 2\},$$  \hspace{1cm} (3.14)

where $\omega(n)$ denotes the approximant of length $n$. In principle, this requires an analysis of the trace of $R_n$ in the limit $n \to \infty$. Taking the Thue-Morse substitution (2.17) as an example, putting $a^{(m)} = \text{tr} (T^{(m)}(a))$ and $b^{(m)} = \text{tr} (T^{(m)}(b))$, then it follows from the relation (3.9) that

$$a^{(m+3)} = \text{tr} (T^{(m+3)}(a)) = \text{tr} (T^{(m+1)}(abba) = \text{tr} (T^{(m+1)}(a))^2(T^{(m+1)}(b))^2),$$

using the fact that the trace is invariant under cyclic permutation of the matrices. Squares can be broken down with the formula

$$M^2 = \text{tr}(M)M - I,$$  \hspace{1cm} (3.15)

which results from an application of the Cayley-Hamilton theorem to an arbitrary matrix $M \in \text{SL}(2,\mathbb{R})$. Repeated use of the relation (3.15) gives

$$a^{(m+3)} = a^{(m+2)}a^{(m+1)}b^{(m+1)} - [a^{(m+1)}]^2 - [b^{(m+1)}]^2 + 2, \hspace{1cm} m \geq 0,$$  \hspace{1cm} (3.16)

which can further be simplified using the equality $a^{(m+1)} = b^{(m+1)}$. For the Thue-Morse model this is a three-dimensional nonlinear map, which is called the trace map. From this map it is easily seen, that if $a^{(m_0+2)} = 2$ for some $m_0$ then $a^{(m+2)} = 2$ for all $m > m_0$, and consequently all energy values for which this is fulfilled belong to the spectrum for every periodic approximant $\mathcal{H}_{\sigma^{m_0+2}(a)}$. This means that the corresponding transfer matrices $T^{(m+2)}(a)$ for $m \geq m_0$ (and analogously for the letter $b$) will be identity matrices and thus commute with each other.
on different length scales giving rise to so-called “lattice-like” states \[140\]. One such example is provided by the lowest energy state in the Thue-Morse model with the implication of a wavefunction showing a three-level structure as depicted in Fig. 3.1(a), which was called Bloch-like when such eigenstates were first found \[134\]. The generic dynamics of the trace map is however chaotic in nature, resulting in irregular wavefunctions, as opposed to the (quasi-)periodic orbits resulting in self-similar wavefunctions. There are also examples for which the wavefunctions appear localized for any finite approximation of the chain as shown in Fig. 3.1(b) for the Rudin-Shapiro model.

In order to use the trace map for the spectral analysis, one needs to relate the spectrum to quantities of the dynamical system induced by the trace map. A suitable definition of a stable set that will contain the spectrum is to define it as the complement of an unstable set, which is (conveniently) chosen as the set for which the absolute value of the trace is larger than two for all \( n \) larger than some fixed value \( n_0 \) \[26\]. Under this condition, one can construct a sequence of periodic approximants \( H_\omega(n) \), converging strongly to \( H_\omega \), which by Floquet theory implies that if \( E \) is in the spectral gap for the periodic approximant, it will be in the gap also for the limiting operator. The corresponding stable set, denoted by \( B_\infty \), is usually called the dynamical spectrum.

For some models it can be shown that the dynamical spectrum \( B_\infty \) coincides with the real spectrum. Using the trace map of the Fibonacci model \[89\], it was shown in 1986 \[31\] that the dynamical spectrum is a Cantor set of zero measure for strong enough values of the potential. In a landmark paper by Sütő \[149\] in 1987, it was proven that the dynamical spectrum coincides with the real spectrum and also that a pure point part of the spectrum is absent. That the spectrum is purely singular continuous and supported on a Cantor set of zero measure was completed in 1989 by the use of Lyapunov exponents \[150\]. An analogous result for the spectrum of the Thue-Morse model has been proven \[21, 42\] using the trace map in Eq. 3.16. A finite approximation of the spectrum for the Thue-Morse model is depicted in Fig. 3.2. In the limit of the infinite lattice the dynamical spectrum coincides with the real spectrum, which is a Cantor set of zero measure. The nowhere dense structure of the spectrum can be illustrated by plotting the inte-
3.2 Spectrum and wavefunctions

Figure 3.2. Electronic spectrum for the Thue-Morse model with the values $V_a = 1$ and $V_b = -1$ of the potential. The number of sites is 65536. The inset shows the integrated density of states (IDOS($E$) as a change of coordinate axis relatively to the main figure) which illustrates the devil’s staircase feature of this function. Courtesy of Lennholm [100].

Integrated density of states, IDOS($E$). It is defined as the number of eigenvalues with an energy $E_n \leq E$, which for a singular continuous spectrum is a monotonously increasing function of the energy which has a derivative that is zero almost everywhere. The qualitative features of such a function (a devil’s staircase) is shown in the inset of Fig. 3.2 for the Thue-Morse model.

For a given primitive substitution $\sigma$ defined on a finite alphabet $\mathcal{A}$, one can always find a trace map by combining the relation (3.9) with the equation [92]

$$\text{tr}(\mathcal{M} \mathcal{N} \mathcal{O}) = \text{tr}(\mathcal{M}) \text{tr}(\mathcal{N}) \text{tr}(\mathcal{O}) + \text{tr}(\mathcal{N}) \text{tr}(\mathcal{O}) - \text{tr}(\mathcal{N}) \text{tr}(\mathcal{O}),$$

(3.17)

which is satisfied when all of the matrices belong to the group $\text{SL}(2, \mathbb{R})$. By defining the trace coordinates $a_i^{(m)} = \text{tr} \left( T^{(m)}(a_i) \right)$, where $a_i \in \mathcal{A}$, there exists a finite set $\mathcal{B} \subset \mathcal{A}$ such that the product of polynomial expressions for the traces at some level $m + 1$ can be expressed in terms of those at level $m$. For the Thue-Morse trace map [84, 10], a suitable choice is seen to be the set $\mathcal{B} = \{ \sigma(a), \sigma(b), \sigma^2(a) \}$. Under the assumption of semi-primitive trace maps (see Paper I, Appendix A, for a definition), Bovier and Ghez [24] obtained a trace map characterization of the spectrum by showing that it is equal to the dynamical spectrum $\mathcal{B}_\infty$ and that it coincides with the set where the Lyapunov exponent vanishes. Building upon these results, Liu et al. [104] showed in the year 2002, that the corresponding induced trace map always can be chosen such that it is semi-primitive, from which it was proven that the spectrum indeed is a Cantor set of zero measure.

The key ingredient for excluding a pure point spectrum is to obtain estimates on the trace map such that for all energies in the spectrum no solution tends to zero at infinity. This can be an outstanding problem, since in most cases the
actual trace map is quite complicated and its analysis very difficult to carry out. In Ref. [25] it has been shown that the absence of eigenvalues is at least guaranteed if the sequence has an ever growing (invariant) square of two identical words. The same conclusion is valid whenever the sequence has a (strongly) palindromic property as shown in Ref. [65]. One example of a substitution sequence that compromises these behaviors is that of the period-doubling model. The spectrum for this model is thus purely singular continuous, as was proved already in Ref. [21], a result that actually holds true on a set of full measure [39]. The illusive Rudin-Shapiro model does not satisfy any of the above mentioned requirements [6, 18]. This model was investigated by Dulea, Johansson, and Riklund [44, 45, 46] a decade ago. Extensive and high precision numerical analyses led to the conjecture that the spectrum is pure point, at least for strong enough values of the potential. For smaller values of the potential (compared to the hopping integral) extended and self-similar wavefunctions were however found, but they seemed to be exceptions, occurring for very special values of the energy. This question is settled by proving the absence of localization in the Rudin-Shapiro model in Paper III.

3.3 Quantum dynamics

The study of the dynamical localization properties is the most appealing approach in determining the physical properties related to the character of the energy spectrum for different lattice models. Here the transport properties of single-site excitations in on-site tight-binding lattices are considered. This concerns the asymptotic behavior of the time-evolution of the electronic wave packet $\psi(t) = e^{-itH}\psi(0)$ for an initial state $\psi(0) = \psi_{n_0}(0)$ localized at site $n_0$ in the lattice at time $t = 0$.

The existence of localization can be verified by computing the probability to find the electron at the initial site $P_{n_0}(t) = |\psi_{n_0}(t)|^2$. Since the probability of return can oscillate and thus not always possess an asymptotic limit, the temporal autocorrelation function

$$C(t) = \frac{1}{t} \int_0^t P_{n_0}(t') dt'$$

is usually studied. It is well known that $\lim_{t \to \infty} C(t) = 0$ if and only if the spectral (local density of states) measure associated with the initial state is continuous [132]. When a pure point part of the spectrum is absent, the function (3.18) has been shown [84] to decay algebraically in time as

$$C(t) \sim t^{-\Delta}, \quad t \to \infty,$$

where $\Delta$ has been proven [33, 20] to be equal to the correlation dimension $D_2$ [63]. When the spectrum is absolutely continuous $D_2 = 1$, while $D_2 = 0$ for pure point spectrum. This gives a possibility of, at least numerically, exclude a pure point part of the spectrum for a given model by showing that the exponent $\Delta > 0$. This measure is used in Paper III to support the absence of localization in the Rudin-Shapiro model, which is in contrast to the conjecture in Ref. [40], where the presence of a pure point spectrum is presented. However, it should be noted
that the asymptotic regime for $C(t)$ is reached very slowly, and that multiscaling in time (quantum intermittency) is likely to be present \cite{62}, because of the fractal-like nature of the energy spectrum.

Figure 3.3. The time evolution of the logarithm of the root-mean-square displacement $[\langle x^2(t) \rangle]^{1/2}$ for an electron, which at time $t = 0$ was localized at site $n_0 = 1024$, in a Rudin-Shapiro lattice of length $N = 2048$. The upper curve corresponds to the potential $V_a = -V_b = 1$, while for the lower curve the potential is $V_a = V_b = \sqrt{2}$.

A measure of the spreading of the electronic wave packet $\psi(t)$ is the mean-square displacement

$$\langle x^2(t) \rangle = \sum_n (n - n_0)^2 |\psi_n(t)|^2. \quad (3.20)$$

When the spectrum contains a continuous part, the asymptotics of $\langle x^2(t) \rangle$ is expected to increase as a power of time according to

$$\langle x^2(t) \rangle \sim t^{2\beta}, \quad t \to \infty, \quad (3.21)$$

where $\beta = 1/2$ for diffusive behavior and $\beta = 1$ for ballistic transport (which is mainly related to absolutely continuous spectrum \cite{148}). Even though the absence ($\beta = 0$) of diffusion is a characteristic feature of random systems \cite{7}, the mere exponential localization of states does not imply dynamical localization \cite{11}. One example being the random dimer model \cite{48} with short-range correlations, which can even show superdiffusive ($\beta > 1/2$) transport. For aperiodic lattices anomalous diffusion, characterized by a scaling exponent $0 < \beta < 1$ is usually found, which is consistent with purely singular continuous spectrum \cite{152}. Figure 3.3 illustrates the different time-scales present in quantum diffusion, where the stronger aperiodic potential tends to give a larger (average) slope $\beta$ but smaller width than for the weaker potential still. Finally, there is in the multifractal framework a hierarchy of generalized dimensions that can be used in estimating the dynamics, of which the
information dimension $D_1$ has been proven to give a bound on the diffusion from below, $D_1 \leq \beta$, and it has also been argued that $\beta$ is related to the multifractal dimensions of both the energy spectrum and the eigenstates.

### 3.4 Mobility edges?

The additive Markov chain offers a possibility to introduce disorder into the ideal deterministic aperiodic structures keeping part of their long-range correlations intact. One of the intriguing questions that comes to mind is whether it is possible to reveal a metal-insulator transition in chains that are built from a finite number of elements. A perturbative approach of the tight-binding Schrödinger equation with a weak binary potential reveals a relation between the Lyapunov exponent $\Lambda$ and the Fourier transform $\hat{K}$ of the two-point correlation function $K(r)$, defined from (2.26). To second order in the perturbation the relation, expressed via the normalized Lyapunov exponent $\Lambda'$, reads

$$\Lambda'(E) = \frac{32 \sin^2(k)}{(\varepsilon_1 - \varepsilon_0)^2} \Lambda = \hat{K}(2k), \quad k \in [-\pi, \pi], \quad (3.22)$$

where the wave number $k$ to zeroth order in the potential $\varepsilon(n) \in \{\varepsilon_0, \varepsilon_1\}$ is related to the energy by the band formula $E = -2 \cos k$. Equation (3.22) enables the design of filters with selective spectral components in characteristic intervals by solving Eq. (2.27) for the correlator $K(r) = \sin(0.9\pi r)/(0.9\pi r)$. From Paper IV.

![Figure 3.4](image.png)

**Figure 3.4.** The normalized Lyapunov exponent $\Lambda'(E)$ versus energy $E$. The solid line is the prescribed characteristic: $\Lambda' = 0$ for $0 < E < 0.4$ and $\Lambda' = 0.77$ for $0.4 < E < 2$. The dots are the result from the calculation of the Lyapunov exponent of the sequence $\varepsilon(n)$ constructed by means of the memory function $F(r)$ with $N = 300$ as a solution of Eq. (2.27) for the correlator $K(r) = \sin(0.9\pi r)/(0.9\pi r)$. From Paper IV.
In this chapter, vibrational properties of some lattice models are described from the viewpoint of classical mechanics. The treatment of elastic vibrations in harmonic chains is discussed, but also the phenomenon of discrete breathers, that is, time-periodic localized solutions in certain anharmonic lattices, is outlined.

4.1 Harmonic lattices

Consider a one-dimensional chain of classical particles with masses \( m_n \), connected by nearest-neighbor springs with spring constants \( k_2 \equiv 1 \). Assuming a simple interaction in the form of a harmonic potential, the Hamiltonian can be written

\[
H = \sum_n \left[ \frac{p_n^2}{2m_n} + \frac{1}{2} (q_n - q_{n-1})^2 \right],
\]

(4.1)

where \( q_n \) is the displacement (from the equilibrium position) of the \( n \)th particle and \( p_n = m_n \dot{q}_n \) denotes its momentum. (For an aperiodic chain both the masses and the spring constants can, of course, be varied simultaneously.) The Hamilton's equations

\[
\dot{q}_n = \frac{\partial H}{\partial p_n}, \quad \dot{p}_n = -\frac{\partial H}{\partial q_n},
\]

(4.2)

applied to the Hamiltonian (4.1) give the equations of motion

\[
m_n \ddot{q}_n(t) = q_{n+1}(t) - 2q_n(t) + q_{n-1}(t),
\]

(4.3)

which alternatively could have been obtained directly from Newton's second law. Separating the time dependence with the Ansatz \( q_n(t) = \xi_n \exp(-i\omega t) \), the equations for the spatial dependence, written in the transfer matrix formalism, become
\[
\begin{pmatrix}
\xi_{n+1} \\
\xi_n
\end{pmatrix} = \begin{pmatrix}
2 - \omega^2 m_n & -1 \\
0 & 1
\end{pmatrix} \begin{pmatrix}
\xi_n \\
\xi_{n-1}
\end{pmatrix} \equiv T_n \begin{pmatrix}
\xi_n \\
\xi_{n-1}
\end{pmatrix}.
\] (4.4)

The transfer matrix \( T_n \) in (4.4) belongs to the group \( SL(2, \mathbb{R}) \) of unimodular matrices and it depends on a single index \( n \). However, this system does not represent a “normal” eigenvalue problem for \( \omega^2 \) because this factor is multiplied with the masses \( \{m_n\} \), which describe the variation in the model.

The generalized eigenvalue problem (4.3) can be put in ordinary form by invoking the canonical transformation

\[
q_n \rightarrow u_n/\sqrt{m_n}, \quad p_n \rightarrow v_n/\sqrt{m_n},
\] (4.5)

which turns the Hamiltonian (4.1) into

\[
H = \sum_n \left[ \frac{v_n^2}{2} + \frac{1}{2} \frac{u_n - u_{n-1}}{\sqrt{m_n}} \right].
\] (4.6)

With an analogous variable separation as \( u_n(t) = \xi^{(m)}_n \exp(-i\omega t) \), the resulting equations of motion in the mass-dependent \( \xi^{(m)}_n = \xi_n \sqrt{m_n} \) variables become

\[
\frac{2}{m_n} \xi^{(m)}_n - \frac{1}{\sqrt{m_n m_{n+1}}} \xi^{(m)}_{n+1} - \frac{1}{\sqrt{m_n m_{n-1}}} \xi^{(m)}_{n-1} = \omega^2 \xi^{(m)}_n,
\] (4.7)

which is of the same form as the mixed tight-binding Schrödinger equation (3.4).

For a system with \( N \) degrees of freedom, putting \( \xi^{(m)} = (\xi^{(m)}_1, \ldots, \xi^{(m)}_N)^T \), these relations can be expressed as \( D \xi^{(m)} = \omega^2 \xi^{(m)} \), where \( D \) is the symmetric dynamical matrix with obvious entries. The properties of the spectra and the eigenstates of aperiodic chains have been extensively studied by numerical methods, see for example, the papers by Salejda [141, 142, 143].

The transfer matrix formulation of the relations (4.7) is obtained by introducing \( \Theta_n = (\xi^{(m)}_{n+1}, \xi^{(m)}_n)^T \), which results in the difference equation \( \Theta_n = \tilde{T}_n \Theta_{n-1} \), where

\[
\tilde{T}_n = \begin{pmatrix}
\sqrt{m_n m_{n+1}} & 0 \\
0 & 1
\end{pmatrix} \begin{pmatrix}
(2/m_n - \omega^2) & -1 \\
1 & 0
\end{pmatrix} \begin{pmatrix}
1 \\
0/\sqrt{m_n m_{n-1}}
\end{pmatrix}
\] (4.8)

is the transfer matrix. \( \tilde{T}_n \) is unimodular if \( m_{n+1} = m_{n-1} \), which is certainly not fulfilled by every matrix in the case of aperiodic distributions of masses \( \{m_n\} \). Moreover, since the matrix \( \tilde{T}_n \) depends on the nearest-neighbor particles it is not obvious whether there is a one-to-one correspondence between the sequence of transfer matrices and the substitution rule governing the distribution of masses. If this is the case, the order between the transfer matrices is the same as the underlying sequence according to which the masses are ordered. Then the nature of the vibrational spectrum is the same as that of the electronic spectrum for the on-site tight-binding Schrödinger equation. This has been proven to be the case for the Fibonacci model [26, 96]. It should be noted that the term phonon spectrum is often used as a synonym for the vibrational spectrum of normal modes.
4.1 Harmonic lattices

Figure 4.1. Vibrational spectrum for a diatomic chain containing $N = 32768$ masses, $m_a = 1$ and $m_b = 2$, distributed according to the Thue-Morse sequence. The inset shows a magnification of one part, which illustrates the tendency towards the dense-gap structure and the self-similarity. With kind permission from Ref. [100].

The appearance of the phonon spectrum is qualitatively different from the electronic case, even though the character of the spectrum can be the same. For an infinite periodic distribution of two different masses like $(\cdots m_a m_b m_a m_b m_a m_b \cdots)$, the vibrational eigenstates are extended throughout the chain, and the spectrum is absolutely continuous. In this case, the vibrational spectrum is characterized by two bands, the acoustic branch and the optical branch, separated by a gap of frequencies for which no solutions exist [10]. On the other hand, a deterministic aperiodic distribution of masses quite generally give a dense set of gaps. This is illustrated in Fig. 4.1 for the Thue-Morse chain (cf. the corresponding electron spectrum in Fig. 3.2). This model is rather rigorously analyzed in [17], where the value of the integrated density of states on each of the gaps is determined. For periodic approximants of the Thue-Morse chain, a countable dense subset of frequencies in the spectrum was found, whose associated eigenstates are extended, because of commuting transfer matrices. It was also shown that the spectrum is a Cantor set, and numerical evidence indicated that it is of zero measure. The absence of eigenvalues in the spectrum is established for a Thue-Morse ordering in Paper II, leading to the conclusion that the phonon spectrum is purely singular continuous and supported on a Cantor set of zero Lebesgue measure. An analogous result is obtained for the period-doubling chain, and for the Rudin-Shapiro ordering using the result from Paper III. One of the fundamental ingredients in establishing results of this kind is to show unimodular invariance of the transfer matrix (4.8) with respect to certain substitution rules, so that the spectral theory outlined in Chapter 3 can be applied. However, there are physical phenomena, like for example thermal expansion, that cannot be described by simple harmonic interactions, indicating the need for turning to anharmonic models.
4.2 Anharmonic lattices

When a physical model of a lattice is limited to linear equations, the discrete translational symmetry must be broken in order to yield spatially localized solutions. Added impurities in a harmonic lattice may give rise to localized modes in the vibrational pattern. However, in 1988 Sievers and Takeno [147] found that it is possible to have time-periodic, exponentially localized modes in lattices without imperfections if the interaction potential has anharmonic terms so that the governing dynamical equations are fundamentally nonlinear. The frequencies of the modes found, which they called intrinsic localized modes, turned out to be larger than the highest allowed frequency value of the corresponding harmonic chain.

The synonymous term discrete breathers for intrinsic localized modes appeared in connection with the description of discrete analogs [28] of the bound state breather solution

$$u(x, t) = 4 \arctan \frac{\sqrt{1 - \omega^2 \sin \omega t}}{\omega \cosh \sqrt{1 - \omega^2 x}}$$

(4.9)

to the integrable sine-Gordon equation $\partial^2 u / \partial t^2 - \partial^2 u / \partial x^2 + \sin u = 0$, which can be viewed as a nonlinear analog of standing waves on an elastic string [1]. Unlike breather solitons in some integrable systems, the discrete breathers are often robust and persist against small model perturbations. But it is of crucial importance that the frequency of the breather, or any of its harmonics does not resonate with the spectrum of linear modes (phonons), in order for the breather to remain localized. Otherwise the breather might excite phonons and energy can be transported away from the localized solution. The limited bandwidth due to the discreteness of a lattice makes this a generic phenomenon of anharmonic lattices since nonlinearity generates frequencies outside the phonon spectrum. Their existence as exact, linearly stable time-periodic solutions has been proven by MacKay and Aubry [108] for a wide class of models close to their anti-continuous limit, corresponding to uncoupled anharmonic oscillators (see also [14] for a variational approach).

The proof makes use of the implicit function theorem [137] for the continuation of periodic orbits from the anti-continuous limit provided that the solution is nonresonant with the linear method. This recipe also provides an efficient method for calculation of discrete breathers, an implementation made use of in Papers V and VI. It is believed that such localized and typically stable nonlinear excitations can play an important role for the dynamics in, e.g., molecular crystals, biomolecules, and polymers. For reviews on the subject of discrete breathers, see Refs. [11, 55, 107, 27]. Although breathers are particular solutions, they show up spontaneously and persist with long life-time in numerical simulations of the dynamics of anharmonic models.

The inclusion of anharmonicity can be made by keeping more terms in a Taylor expansion of the coupling potential $V(u_n - u_{n-1})$, e.g., by adding the terms

$$V_{k_3 k_4} = \sum_n \left[ \frac{k_3}{3} \left( \frac{u_n}{\sqrt{m_n}} - \frac{u_{n-1}}{\sqrt{m_{n-1}}} \right)^3 + \frac{k_4}{4} \left( \frac{u_n}{\sqrt{m_n}} - \frac{u_{n-1}}{\sqrt{m_{n-1}}} \right)^4 \right]$$

(4.10)

to the harmonic ($k_2 = 1$) potential in the Hamiltonian (4.6). In view of the canonical transformation [140] the conjugate momentum is $p_n = \dot{u}_n$, so that Hamilton’s
4.2 Anharmonic lattices

Equations of motion can be written in compact form as

\[ \dot{\eta} = \mathcal{J} \frac{\partial H}{\partial \eta} \equiv \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \{\partial H/\partial u_n\} \\ \{\partial H/\partial v_n\} \end{pmatrix} = F(\eta) \] (4.11)

for the phase-space coordinates \( \eta = (u, \dot{u}) = (\{u_n\}, \{v_n\}) \). The antisymmetric matrix \( \mathcal{J} \) is composed of the zero \( 0 \) and identity \( I \) square matrices. A time-periodic solution to the equations of motion can generally be seen as a fixed point of a linear Floquet operator. Indeed, adding a small perturbation \( \epsilon(t) = (\{\epsilon_n\}, \{\dot{\epsilon}_n\}) \) to a solution \( \eta(t) \) one obtains \( F(\eta + \epsilon) \approx F(\eta) + \partial F(\eta)\epsilon \) to first order in the perturbation. Integrating the linearized equation of motion \( \dot{\epsilon} = \partial F\epsilon \) one period of time \( t_\omega = 2\pi/\omega \) gives the Floquet (monodromy) matrix \( M_\omega(\eta) \), defined through

\[ \epsilon(t_\omega) = M_\omega \epsilon(0), \] (4.12)

where \( \omega \) denotes the frequency of the oscillating solution. The symplectic nature of the Floquet matrix \( M_\omega \) implies that if \( \lambda \) is an eigenvalue (Floquet multiplier), so are \( 1/\lambda, \lambda^* \) and \( 1/\lambda^* \), where \( \lambda^* \) is the complex conjugate of \( \lambda \) [135]. A solution is said to be linearly stable if the dynamical perturbation does not grow exponentially in time, which is achieved if all eigenvalues are located on the complex unit circle [114]. This is however no guarantee for the true breather stability, since the solution may appear or disappear spontaneously, interact with other breathers and there are no conservation rules as in integrable systems.

From a known fixed point \( \eta \) to the Floquet operator \( M_\omega \), the iteration

\[ \eta^{(j+1)}(0) = \eta^{(j)}(0) + (I - M_\omega)^{-1}[M_\omega \eta^{(j)}(0) - \eta^{(j)}(0)], \quad j \geq 0 \] (4.13)

of an initial guess \( \eta^{(0)} \) of a “new solution” is performed until it becomes a fixed point to the Floquet operator (within a desired accuracy). This Newton scheme can be used iteratively to trace solution curves in parameter space of the model and perform a stability analysis at the same time. By restricting the dynamics of the Hamiltonian system to time-reversible solutions with zero initial velocity \( \dot{u} = 0 \), in the reduced phase-space \( u(t) = u(-t) \) the singularity of the operator \( (I - M_\omega) \) can be avoided [32, 105, 114]. Then the self-consistent method continues until the discrete breather disappears or a bifurcation is reached.

The description of an uncoupled atom (with mass \( m_a = 1 \)) can effectively be achieved in a diatomic chain if the masses, \( m_b \), of neighboring atoms turn toward infinity. The solution to this integrable system with one characteristic frequency \( \omega \) for a hard \( V_{k_2k_3k_4} = V_{101} \) potential can be expressed in terms of a Jacobi elliptic function [105]. Now, using \( 1/\sqrt{m_b} \) as a parameter in the iteration (4.13) one can find discrete breathers for smaller values of the mass, \( 0 < 1/\sqrt{m_b} \leq 1 \), provided that no harmonics resonate with the linear modes and no bifurcation is encountered. The solution shown in Fig. 4.2(a) is a result of such a continuation in a diatomic Rudin-Shapiro chain with 128 atoms and frequency \( \omega = 2.1 \) to the value \( m_b = 1 \). The explanation for being able to reach a monoatomic chain is that the frequency \( \omega \) lies above the phonon spectrum, which is bounded as \( 0 \leq \omega_0 \leq 2 \).

While tracing solutions from the anti-continuous limit to smaller values of the mass difference the Floquet eigenvalues \( \lambda \) move in the complex plane. If no discrete
breather is excited in the chain, the arguments obey the dispersion relation \[ \arg(\lambda) = \pm \frac{2\pi\omega_0(1/\sqrt{mb})}{\omega} \mod 2\pi, \] (4.14)
where \(\omega_0(1/\sqrt{mb})\) belong to the spectrum of the harmonic chain. With a breather present in the system eigenvalues “escape” from the relation (4.14) and they can produce instabilities through eigenvalue collisions. In Fig. 4.2(b) a pair of eigenvalues has collided at \(\lambda = 1\) and left the complex unit circle, which occurred just before the breather reached a monoatomic chain \((mb = 1)\). The appearance of instabilities can be made clearer by studying the Krein signature \[ \kappa(\lambda) = \text{sign}(\mathcal{J}M, \zeta, \zeta), \] (4.15)
being the definite sign of a scalar product \((\cdot, \cdot)\) associated with a complex eigenvector \(\zeta\) of the conjugated eigenvalues \(\lambda\) and \(\lambda^*\), such that \(|\lambda| = 1\) and \(\lambda \neq \pm 1\). Only colliding eigenvalues with opposite Krein signature can result in instabilities. If the eigenvectors belong to different symmetry classes stability is however preserved [113]. This theory is valid in all essential parts also for infinite chains [109].

The existence of breathers has been shown for monoatomic [72] and diatomic periodic chains [105, 106]. Calculations of breathers from an anti-continuous limit have been performed in, e.g., periodic [37, 159, 111], aperiodic [69] and disordered lattices [93, 94]. The presence of multibreathers, corresponding to several excitations, opens up for the possibility of energy transport in disordered systems [93]. In this context, one should mention that already in 1955 Fermi, Pasta, and Ulam [54] studied numerically the Hamiltonian (4.6) with additional anharmonic terms in the potential, which since then are abbreviated FPU lattices. Contrary to an expected thermalization of the system, they found a recurrence phenomenon of the dynamics where the system after some time returned to a state close to the initial condition. This was the first time a “soliton” [156] revealed itself in a study of a lattice. Its seemingly nonergodic property has strongly influenced the development of the theory of chaos and solitons [29] (and references therein).
An effect of correlation due to electron-lattice interaction can be accounted for by adding a cubic nonlinear term to the tight-binding Schrödinger equation (3.4)

$$V_n \psi_n - \varepsilon (\psi_{n+1} + \psi_{n-1}) + \gamma |\psi_n|^2 \psi_n = E \psi_n,$$

where $E$ is the energy and the (negative) hopping matrix elements $-t_{n,n \pm 1}$ are set equal to a (coupling) constant $\varepsilon$. The on-site potential is again denoted by $V_n$ and $\gamma$ is an anharmonic parameter. In the Holstein model for polarons in molecular crystals the nonlinear term describes the static short-range electron-phonon interaction with $\gamma < 0$ [67, 154]. Another application of Eq. (5.1) is for models of nonlinear optical response of dielectric or magnetic superlattices [82]. The time-independent Eq. (5.1) can be seen as a stationary, $\Psi_n(t) = \psi_n \exp(-iEt)$, analog of the discrete nonlinear Schrödinger equation (DNLS)

$$i \dot{\Psi}_n = V_n \Psi_n - \varepsilon (\Psi_{n+1} + \Psi_{n-1}) + \gamma |\Psi_n|^2 \Psi_n,$$

where the dot means the derivative with respect to time $t$. This is actually a special case of a more general equation, namely the discrete self-trapping equation [51].

The reader is referred to Refs. [52, 85, 50, 123] for fundamental properties of the DNLS equation and its main applications. Despite its simplicity, it is successful in describing coherent structures in such diverse areas as in the Davydov (soliton) model for transport in proteins [144], in models for coupled waveguides arrays in nonlinear media [33, 53, 141], in nonlinear photonic crystals [118], and Bose-Einstein condensates trapped in optical lattices [153]. In this view, results from studies of the DNLS equation as it stands can have bearing on a variety of applications. The importance of the model [52] can also be accentuated by the fact that it generically gives an approximate description of the dynamics of small-amplitude excitations in general anharmonic (Klein-Gordon) lattices [88, 86, 119]. The problem of a periodic modulation potential $V_n$ is addressed in the Papers V and VI.
The DNLS equation (5.2) can be derived from the Hamiltonian
\[ H(\{\Psi_n\}, \{i\Psi^*_n\}) = \sum_n \left[ V_n |\Psi_n|^2 - \varepsilon (\Psi_n \Psi^*_{n-1} + \Psi^*_n \Psi_{n-1}) + \frac{\gamma}{2} |\Psi_n|^4 \right], \tag{5.3} \]
using the conjugated variables \( q_n \equiv \Psi_n \) and \( p_n \equiv i \Psi^*_n \) in (4.2). In addition to the Hamiltonian energy, also the norm (excitation number), defined by
\[ N = \sum_n |\Psi_n|^2, \tag{5.4} \]
is a conserved quantity for the system (5.2). The integrability for the case of two sites, i.e., \( n \in \{1, 2\} \), can be expressed in terms of elliptic functions \[76\]. Otherwise, complete integrability is only recovered in the continuous limit
\[ i \frac{\partial \Psi}{\partial t} = [V(x) - 2\varepsilon] \Psi - \varepsilon \frac{\partial^2 \Psi}{\partial x^2} + \gamma |\Psi|^2 \Psi, \tag{5.5} \]
where the nonlinear Schrödinger (NLS) equation for a constant potential \( V(x) \equiv 2\varepsilon \) (without loss of generality for the particular choice) has an infinite set of conserved quantities \[157, 158, 43\]. One may note that the transformation \( \Psi \to \sqrt{\varepsilon} \Psi, \ V \to \varepsilon V, \ t \to t/\varepsilon \) can be used to normalize the coupling \( \varepsilon > 0 \) to unity in the Eqs. (5.1) and (5.5). Then, for \( \gamma < 0 \), the NLS equation has the envelope soliton solution
\[ \Psi(x, t) = C \text{sech} [\alpha(x - \nu t - x_0)] \exp i \frac{\pi}{2}(x - \nu t) + i (\alpha^2 + \frac{\varepsilon^2}{4}) t \tag{5.6} \]
moving with arbitrary velocity \( \nu \). When normalized to unity the amplitude of the soliton is \( C = \sqrt{\alpha/2} \), where \( \alpha = |\gamma|/4 \) is related to the width of the “bell-shaped” function \( \text{sech}(x) = 1/\cosh(x) \) centered around the coordinate \( x_0 \) at \( t = 0 \). The envelope of the minimal-energy stationary soliton reduces to the expression
\[ \psi(x) = \frac{C}{\cosh[\alpha(x - x_0)]}. \tag{5.7} \]
The case of \( \gamma < 0 \) is usually referred to as the focusing equation since the nonlinear term tends to compress an already localized excitation. For a positive \( \gamma \) on the other hand the nonlinear term defocuses a localized structure, but still a solution in the form of a dark soliton \( \psi(x) = C \tanh[\alpha(x - x_0)] \), appearing as a “localized” dip in a constant background, is possible \[87\]. If the magnitude of the parameter \( \gamma \) is small the discrete analogs are well approximated by these solutions and they may be called stationary (discrete) lattice solitons.

5.1 The dispersion relation and standing waves

Inserting a traveling plane wave \( \Psi_n = \psi \exp i(kn - \omega t) \) into equation (5.2) with the constant potential \( V_n = 2\varepsilon \) yields the nonlinear dispersion relation
\[ \omega(k) = 4\varepsilon \sin^2 \frac{k}{2} + \gamma |\psi|^2, \tag{5.8} \]
where the wave numbers $k$ are determined by the boundary conditions. From this relation, the group velocity $\nu_g$ and its dispersion coefficient $D_g$ are found as

$$\nu_g = \frac{\partial \omega}{\partial k} = 2\varepsilon \sin k, \quad D_g = \frac{\partial \nu_g}{\partial k} = 2\varepsilon \cos k.$$  \hfill (5.9)

This implies that a wave with $k = \pi/2$ has maximum velocity and no dispersion, being a pure consequence of the discreteness of the lattice. (In the continuous case, the unbounded dispersion relation $\omega = \varepsilon k^2 + \gamma |\psi|^2$ gives $\nu_g = 2\varepsilon k$ and $D_g = 2\varepsilon$, being approximately equal to (5.9) for $k$ small.) Linear stability of solutions, as discussed in Section 4.2, can be analyzed in the rotating-wave frame, realizing the splitting of plane waves through modulational instabilities.

Continuations of linear standing waves (of the form $\cos(kn + \beta)$) into the nonlinear regime, also exist and define nonlinear standing waves $\psi_n \exp(-i\omega t)$, although they cannot be written as linear combinations of counter-propagating waves $\exp(\pm ikn)$ due to the absence of superposition principle. In particular, close to the linear limit (corresponding to $\gamma \to 0$ in Eq. (6.8)) all nonlinear standing waves with $k \neq \pi$ are unstable for infinite systems. Because of a second conserved quantity, a curve relating the Hamiltonian and norm densities according to $H/N = \gamma (N/N)^2$, where $N$ is the lattice size, has been found to divide the phase space into two regions with qualitatively different asymptotic dynamics. On one side ($|k| > \pi/2$) of the curve, which coincides with the nonlinear standing wave with $k = \pi/2$, the system shows thermalization according to the Gibbsian equilibrium distribution. A discontinuity in the partition function signals a phase transition in the other region ($|k| < \pi/2$) where statistical localization is favorable. Studies of the dynamics in this regime typically reveal the spontaneous formation of intrinsic localized modes – discrete breathers.
5.2 Stationary and non-stationary solutions

A stationary time-periodic solution, \( \Psi_n(t) = \psi_n \exp(-i\omega t) \), inserted into Eq. (5.2), yields the asymptotic solutions

\[
|\psi_n|^2 = (\omega - V_n)/\gamma
\]

in the anti-continuous limit \( \varepsilon/\omega \to 0 \), from which particular configurations can be (numerically) traced through parameter space \[51, 108, 50, 112\]. It is important to notice that there are restrictions on the choice of asymptotic codes in order to obtain stationary time-periodic solution. For example, if two equivalent sites are excited with incommensurate frequencies (different amplitudes) the solution is not stationary anymore, but rather quasiperiodic in time. Non-stationary solutions of this form can be obtained from the Ansatz

\[
\Psi_n(t) = \psi_n(t)e^{-i\omega t}, \tag{5.11}
\]

where the time-dependence of the amplitude \( \psi_n(t) \) is not harmonic. Again, because of the second conserved quantity \( \delta \), quasiperiodic solutions with two frequencies with irrational quotient exist in continuous families \[108, 78, 19\]. For an aperiodic modulation \( V_n \) one might expect that solutions with more than two frequencies can survive for the infinite system. But then again, the equation is not integrable so also chaotic behavior should appear for typical initial conditions \( \psi_n(t) \). There is also an interesting discussion about \textit{intraband discrete breathers} in disordered systems \[94\]. When nonresonant with the linear Anderson modes these breathers exist inside the point spectrum, suggesting that the set of allowed frequencies for the localized solutions becomes a (fat) Cantor set of non-zero measure in the limit of an infinite system. The existence of both time-periodic \[4\] and quasiperiodic \[56\] localized solutions in disordered lattices has been proven.

In the Papers V-VI, an understanding for the case with a periodic potential \( V_n = (-1)^n V_0 \) is developed. Particular emphasis is put on the formation and persistence of the fundamental discrete gap soliton as the energetically favorable stationary state in the spectral gap. The ground state should be the “ordinary” discrete soliton bifurcating from the (lower band edge) weakly nonlinear standing wave with wave number \( k = 0 \). The time-development of the modulational instability for this solution, found by numerical integration of the DNLS equation \( \delta \), is depicted in Fig. 5.1 (cf. Fig. 1.5 for \( k = \pi/2 \) and the creation of the gap soliton). The unstable modulations along the lattice develop into a number of excitations that begin to perform translational motion and they interact in the typical manner of colliding discrete solitons. In time, the small excitations typically coalesce into a reduced number of larger structures that become rather immobile with growing amplitudes. The energy in the intrinsically localized modes continue to grow at expense of the kinetic energy of the phonons \[79, 129\]. A guess based on physical intuition could be that only one localized mode remains in the long-time limit. However, awaiting the appearance of the ground state this thesis would perhaps never have been finished.
Bibliography


[127] Pisano L (Fibonacci), Liber Abbaci (1202).


[156] Zabusky N, Kruskal M, Interaction of “solitons” in a collisionless plasma and

and one-dimensional self-modulation of waves in nonlinear media, Zh. Eksp.

[158] Zakharov V E, Shabat A B, Interactions between solitons in a stable medium,

[159] Zolotaryuk A V, Maniadis P, Tsironis G P, Discrete gap breathers in chains
A.1 Paper V

- Equation (3) on the article page number 641 should read

\[
\begin{align*}
(\omega - \omega_0^{(n)} + 2\varphi_n^2)\alpha_n + \alpha_{n+1} + \alpha_{n-1} + \varphi_n^2\beta_n &= -\Omega\alpha_n, \\
(\omega - \omega_0^{(n)} + 2\varphi_n^2)\beta_n + \beta_{n+1} + \beta_{n-1} + \varphi_n^2\alpha_n &= \Omega\beta_n.
\end{align*}
\]

- The dot marked by 4 on the smooth solution curve \(\omega_c(N)\) for the gap-out-gap soliton in Fig. 2 is not a bifurcation point.