Wave transmission in nonlinear lattices

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WAVE TRANSMISSION IN NONLINEAR LATTICES

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Abstract

The interplay of nonlinearity with lattice discreteness leads to phenomena and propagation properties quite distinct from those appearing in continuous nonlinear systems. For a large variety of condensed matter and optics applications the continuous wave approximation is not appropriate. In the present review we discuss wave transmission properties in one dimensional nonlinear lattices. Our paradigmatic equations are discrete nonlinear Schrödinger equations and their study is done through a dynamical systems approach. We focus on stationary wave properties and utilize well known results from the theory of dynamical systems to investigate various aspects of wave transmission and wave localization. We analyze in detail the more general dynamical system corresponding to the equation that interpolates between the non-integrable discrete nonlinear Schrödinger equation and the integrable Albowitz–Ladik equation. We utilize this analysis in a nonlinear Kronig–Penney model and investigate transmission and band modification properties. We discuss the modifications that are effected through an electric field and the nonlinear Wannier–Stark localization effects that are induced. Several applications are described, such as polarons in one dimensional lattices, semiconductor superlattices and one dimensional nonlinear photonic band gap systems. © 1999 Elsevier Science B.V. All rights reserved.

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1. Nonlinear lattice systems

1.1. Introduction

Nonlinear lattices are formed when physical properties of a system are described through an infinite set of coupled nonlinear evolution equations. The lattice has typically spatial connotation since, in most cases of interest, the physical system corresponds to coupled sets of linear or nonlinear oscillators distributed in space. If we are interested in phenomena with a length scale much larger than the typical distance between the oscillators, we can perform a continuous approximation and obtain nonlinear partial differential equations. Many of these equations that result from this continuous approximation have interesting properties and lead to solitons, solitary waves, breathers, etc. The other limit where the waves of interest are in the same scale of the typical interoscillator distance is also quite interesting and the corresponding wave properties are quite distinct from those in the continuous limit. In this realm nonlinearity and discreteness conspire into producing localized modes as well as global lattice properties different from those of the continuous model. The emphasis of this review will be towards describing global lattice properties related to wave transmission through one dimensional discrete nonlinear systems. We will use as our paradigmatic equation for this review a generalized version of the discrete nonlinear Schrödinger (DNLS) equation that contains both integrable and nonintegrable terms. A major part of the review will deal with a nonlinear version of the Kronig–Penney model with delta functions, or a nonlinear Dirac comb, that will be shown to be equivalent to a DNLS-like nonlinear lattice.

1.2. The discrete nonlinear Schrödinger equation

The DNLS or discrete self-trapping equation (DST) describes properties of chemical, condensed matter as well as optical systems where self-trapping mechanisms are present. These mechanisms arise either from strong interaction with environmental variables or genuine nonlinear properties of the medium. The DNLS equation was introduced in order to describe the dynamics of a set of nonlinear anharmonic oscillators and to understand nonlinear localization phenomena [1]. It can also be viewed as an equation describing the motion of a quantum mechanical particle interacting strongly with vibrations [2]. If $\psi_n(t)$ denotes the probability amplitude for the particle to be at site $n$ of a one dimensional lattice at time $t$, DNLS reads:

$$i\frac{d\psi_n}{dt} = \varepsilon_n\psi_n + V(\psi_{n-1} + \psi_{n+1}) - \gamma|\psi_n|^2\psi_n,$$

(1)

where $\varepsilon_n$ designates the local energies at site $n$ of a one dimensional crystal, $V$ is the nearest-neighbor wavefunction overlap and $\gamma$ is the nonlinearity parameter that is related to the local interaction of the particle with other degrees of freedom of the medium. Typically an infinite, discrete set of equations, such as DNLS, is viewed in two different ways, either as a discretization of a corresponding continuous field equation, or an equation describing dynamics in discrete geometries. In the case of DNLS, the corresponding continuous field equation is the celebrated nonlinear Schrödinger equation. The present exposition will take the point of view that DNLS represents dynamics in a discrete one dimensional lattice. We will therefore not relate properties of DNLS with the corresponding continuous equation.
The DNLS equation has a long history; in its time independent form was first obtained by Holstein in his study of the polaron problem [3]. Subsequently derived in a fully time-dependent form by Davydov in his studies of energy transfer in proteins and other biological materials [4–7]. Eilbeck, Lomdahl and Scott [1,8–10] studied DNLS as a Hamiltonian system of classical oscillators, focused on analytical and perturbative results and showed that bifurcations occur in the space of stationary states for different values of the nonlinearity parameter. These bifurcations in the discrete set of equations are associated with the nonlinearity induced self-trapping described by DNLS. In order to understand the dynamical properties of DNLS solutions, Kenkre, Campbell and Tsironis studied extensively the nonlinear dimer, the smallest nontrivial DNLS unit [2,11,12]. The latter proved to be completely integrable and from its complete solution a number of interesting properties of self-trapping were obtained. Additionally, the effects of nonlinearity on a variety of physical observables were studied leading to predictions for possible experiments [13–15].

By adding to the DNLS equation a nonlinear term that is identical to the one in the Ablowitz–Ladik (AL) [16] equation one obtains a combined AL-DNLS equation [17,18]:

\[ i \frac{d\psi_n(t)}{dt} = (1 + \mu |\psi_n(t)|^2)[\psi_{n+1}(t) + \psi_{n-1}(t)] - \gamma |\psi_n(t)|^2 \psi_n(t), \]  

where we set for simplicity \( \varepsilon_n = 0 \). We note that for \( \gamma = 0 \) Eq. (2) reduces to the integrable Ablowitz–Ladik equation whereas in the other extreme when \( \mu = 0 \) it becomes the nonintegrable DNLS. The combined AL-DNLS equation interpolates between these two extreme cases. In this article we will deal almost exclusively with stationary properties of DNLS and DNLS-like equations, such as the AL-DNLS equation, in extended lattice systems. Since our interest in these problems is motivated through physical applications we will first discuss the context in which DNLS arises in applications.

1.3. The Holstein model and the DNLS

In order to see the connection of DNLS with the Holstein model [3] for molecular crystals we start with the Hamiltonian:

\[
H = \frac{K}{2} \sum_n u_n^2 + (1/2)M \sum_n \left( \frac{du_n}{dt} \right)^2 + \sum_n \varepsilon_n |n\rangle \langle n| - J \sum_n [n + 1] \langle n| + |n\rangle \langle n + 1|]
\]

\[- A \sum_n u_n |n\rangle \langle n|.\]  

(3)

This Hamiltonian represents an excitation moving in a one-dimensional crystal while interacting with local Einstein-type oscillators. In Eq. (3) \( \varepsilon_n \) represents the local site energy at site \( n \), \( J \) gives the magnitude of the wavefunction overlap of neighboring sites, \( |n\rangle \) and \( \langle n| \) are related to the probability amplitudes at site \( n \) whereas \( u_n \) is the displacement of the \( n \)-th local oscillator. The exciton-phonon coupling term is diagonal in the \( |n\rangle \) basis and depends only on local oscillator displacements. If we neglect the kinetic energy terms and expand the time-dependent wave function as \( |\Psi\rangle = \sum_p \Psi_p |p\rangle \), where the \( |p\rangle \) represent Wannier states. Inserting this into the time-dependent Schrödinger equation \( i(d|\Psi\rangle/dt) = H|\Psi\rangle \), and using the orthonormality property for the \( |p\rangle \)'s,
we obtain:

\[ \frac{id\Psi_n}{dt} = \left( \frac{K}{2} \right) \sum_m u_m^2 \Psi_n + \varepsilon_n \Psi_n - J[\Psi_{n-1} + \Psi_{n+1}] - Au_n \Psi_n. \]  

Next, we eliminate the vibrational degrees of freedom by imposing the condition of minimization of the energy of the stationary states [3]. Inserting \( \Psi_n \sim \exp[iEt] \) and using the normalization condition for the amplitudes \( \Psi_n, \sum_p |\Psi_p|^2 = 1 \), we get

\[ E = \left( \frac{K}{2} \right) \sum_n u_n^2 + \sum_n \left[ \varepsilon_n - Au_n \right] |\Psi_n|^2 - J \sum_n \left( \Psi_{n-1} - \Psi_{n+1} \right) \Psi_n^*. \]  

Imposing the extremum energy condition, i.e. \( dE/du_n = 0 \), we obtain \( u_n = A|\Psi_n|^2/K \). Inserting this back into Eq. (4), we get

\[ \frac{id\Psi_n}{dt} = \left( \frac{A^2}{2K} \right) \sum_p |\Psi_p|^4 + \varepsilon_n \Psi_n - J[\Psi_{n-1} + \Psi_{n+1}] - \left( \frac{A^2}{2K} \right) |\Psi_n|^2 \Psi_n. \]  

This last step represents a departure from the Holstein adiabatic approach being valid in a limit where the assumed classical vibrational degrees of freedom adjust rapidly to the excitonic motion. In this anti-adiabatic limit, it is still possible to retain approximately the dynamics in the original Eq. (4). The quantity \( \left( \frac{A^2}{2K} \right) \sum_p |\Psi_p|^4 \) represents the total vibrational energy. If we measure energies with respect to this background value, we arrive at an effective nonlinear equation for the amplitude \( \Psi_n(t) \):

\[ \frac{id\Psi_n}{dt} = \varepsilon_n \Psi_n - J[\Psi_{n-1} + \Psi_{n+1}] - \left( \frac{A^2}{2K} \right) |\Psi_n|^2 \Psi_n. \]  

This closed nonlinear equation describes the effective motion of the “polaron” in the aforementioned anti-adiabatic limit. The “time step” \( dt \) in the time derivative should be understood as short compared to the time scale of the “bare exciton motion” (proportional to \( 1/J \)) but long compared to the fast vibrational motion (proportional to \( 1/K \)).

1.4. Coupled nonlinear wave guides and the DNLS

In the previous section we showed how DNLS can be motivated in a solid-state context. In an optics context, DNLS describes wave motion in coupled nonlinear waveguides. When an electromagnetic wave is sent through a nonlinear waveguide coupled to other waveguides in its vicinity, \( \Psi_n \) represents the amplitude coefficient in an expansion of the electromagnetic field in terms of the wave normal modes in the waveguide. Coupling causes power to be exchanged among the waveguides. The nonlinear nature of the materials in each waveguide (coupler) can cause a “trapping” of power in one of the waveguides. Self-trapping now happens in space rather than in time. These features could be exploited in the design of optical ultrafast switches with applications in optical computers [19,20].

Nonlinear couplers arranged in various geometries are known to have properties that make them attractive candidates for all optical switching devices. In Fig. 1 we show a typical configuration for an array of such couplers. The basic nonlinear coupler model, introduced by Jensen in 1982, involves two waveguides made of similar optical material embedded in a different host material [19]. The waveguides have strong nonlinear susceptibilities whereas the host is made out
of material with a purely linear susceptibility. The host enables interaction between the modes propagating in the two waveguides whereas the nonlinear susceptibility gives rise to the phenomenon of mode self-trapping in each waveguide. For a device of a given length, the launching of power in one side of the device can give a wide range of amplitudes in each guide. For sufficiently large values of power, the nonlinear susceptibility terms dominate and we have almost complete self-trapping of the energy in the initially excited guide. Switching is possible for a variety of different initial electric field amplitudes in both waveguides [19,21].

We assume an extended system involving many couplers distributed as in Fig. 1 and perform normal mode analysis. From [19], the amplitude $a_{n,\mu}^{(n)}$ of the $\mu$th mode of the $n$th guide, obeys the equation

$$-\frac{i}{4P_{\mu}} \frac{d}{dz} a_{n,\mu}^{(n)} = \oint dx \, dy \, E_{\mu}^{(n)*} \cdot E_{\mu}^{(n)},$$

where the axes of the guides are along $z$, $E_{\mu}^{(n)}$ is the electric field of the $\mu$th mode in the $n$th guide, $P_{\mu}$ is the power in the $\mu$th mode and $P'$ is the perturbing polarization due to linear and nonlinear effects. For the $n$th guide,

$$P'/\varepsilon_0 = E^{(n)} \delta + (\delta + \varepsilon)[E^{(n+1)} + E^{(n-1)}] + \chi^{(3)}[|E^{(n)}|^2 + |E^{(n-1)}|^2 + |E^{(n+1)}|^2]E^{(n)},$$

in which $\varepsilon$ is the dielectric coefficient of the host material, $\varepsilon + \delta$ that of the guide material and $\chi^{(3)}$ is the third-order susceptibility [22]. $E^{(i)}$ is the total field due to the $i$th guide. Eq. (8) then gives

$$-\frac{i}{4P_{\mu}} \frac{d}{dz} a_{n,\mu}^{(n)} = \frac{\alpha \varepsilon_0}{4P_{\mu}} \oint dx \, dy \, \delta E_{\mu}^{(n)*} \cdot E^{(n)} + (\varepsilon + \delta)E_{\mu}^{(n)*} \cdot (E^{(n-1)} + E^{(n+1)})$$

$$+ \chi^{(3)}(|E^{(n)}|^2 + |E^{(n-1)}|^2 + |E^{(n+1)}|^2)(E_{\mu}^{(n)*} \cdot E^{(n)}).$$
Similar equations hold for guides \((n - 1)\) and \((n + 1)\). Expanding the total fields in normal modes, Eq. (10) gives a set of mode-coupled equations for the mode amplitudes. If we assume only the lowest single-mode operation for each guide, so that \(E^{(n)} = d^{(n)}_{\mu}E^{(n)}_{\mu}\) etc. for \(E^{(n-1)}\) and \(E^{(n+1)}\), then Eq. (10) with \(\mu = 1\), gives the following set of equations:

\[
- \mathbf{i} \frac{d_1^{(n)}}{dz} = Q_1^{(n)}d_1^{(n)} + Q_{n,n-1}^{(n)}d_1^{(n-1)} + Q_{n,n+1}^{(n)}d_1^{(n+1)} + Q_3^{(n)}|d_1^{(n)}|^2 d_1^{(n)}. \tag{11}
\]

The coefficients are given by

\[
Q_1^{(n)} = \frac{\alpha E_0}{4P} \int dx \, dy \, \delta|E^{(n)}|^2, \tag{12}
\]

\[
Q_3^{(n)} = \frac{\alpha E_0}{4P} \chi^{(3)} \int dx \, dy \, \delta|E^{(n)}|^4, \tag{13}
\]

\[
Q_{nl} = \frac{\alpha E_0}{4P} \int dx \, dy (\varepsilon + \delta)|E^{(n)}|^2 E^{(l)}, \quad (n \neq l). \tag{14}
\]

The coupling coefficient \(Q_{nl}\) for \(n \neq l\) is generally complex due to the phase mismatch associated with the assumed mode factor \(\exp(\mathbf{i} \beta_\mu z)\). The latter factor enters in a normal mode expansion

\[
E^{(n)} = \sum_\mu d^{(n)}_{\mu} \exp(\mathbf{i} \beta_\mu z) E^{(n)}_{\mu}
\]

for each mode, with \(\beta_\mu\) being the wave vector of propagation of the \(\mu\)th mode propagating in the \(z\) direction. The inner product in the integrand of Eq. (14) may be positive or negative depending on the polarization direction in each waveguide respectively. In the general case of dissimilar waveguides (say guides \(n\) and \(n - 1\)) phase mismatch will result in spatially modulated \(Q_{n,n-1}\) terms proportional to \(\exp(\mathbf{i} \Delta \beta z)\), with \(\Delta \beta\) the difference of the wavevectors of the waves propagating in the two waveguides respectively. When the waveguides are taken to be identical, \(\Delta \beta = 0\) and space modulation is not present. Additionally, with the present boundary conditions at \(z = 0\), the inner product in Eq. (14) is positive and as a result \(Q_{n,n-1}\) is real and positive. If, on the other hand, phase mismatch leads to a spatial \(Q_{n,n-1}\) modulation much faster than the mode amplitude change over the length of the waveguide, an average effective \(Q_{n,n-1}\) can be used. An average of a rapidly oscillating factor \(\exp(\mathbf{i} \Delta \beta z)\) over the device length \(L\), in general to a complex \(Q_{n,n-1}\) term, whose actual value depends on the product \((\Delta \beta)L\). In this context, it is possible to choose values of \(\Delta \beta\) that give rise to a real but negative effective \(Q_{n,n-1}\) term resulting in more abrupt switching properties. Taking \(Q_{n,n-1}\) real, then \(Q_{n,n-1} = Q_{n,n-1, real}\) and by symmetry then \(Q_{n,n+1} = Q_{n+1,n, real}\). Defining \(Q_{n,n-1} = Q_{n,n+1} = - V\), Eq. (11) can now be written as

\[
- \mathbf{i} \frac{d_1^{(n)}}{dz} = Q_1^{(n)}d_1^{(n)} - V(d_1^{(n-1)} + d_1^{(n+1)}) + Q_3^{(n)}|d_1^{(n)}|^2 d_1^{(n)}, \tag{15}
\]

where the subscript 1 in the variables \(d_1^{(n)}\) was dropped. Now letting

\[
d^{(n)} = c_n \sqrt{P} \exp(\mathbf{i} \Omega z), \tag{16}
\]
where $P$ is the total input power and $\gamma = Q_3 P$ gives the simplified equations

$$i \frac{dc_n}{dz} = V(c_{n+1} + c_{n-1}) - \gamma |c_n|^2 c_n. \quad (17)$$

We recognize the DNLS with the standard unity normalization condition

$$\sum_p |c_p|^2 = 1. \quad (18)$$

We note that by normalizing the variables $c(z)$ to one, we can associate each of them with a probability amplitude. We can thus consider DNLS as an effective equation describing the motion (when $z$ is interpreted as "time") of a quantum mechanical particle in a lattice while interacting strongly with other degrees of freedom.

Furthermore, since the nonlinearity parameter $\gamma$ is formally proportional to the total input power $P$, we can express the dependence of coupler properties on $P$ equivalently as the influence of the value of $\gamma$ on the "probability" $|c(z)|^2$. For the nonlinear optical couplers the nonlinear parameter $\gamma$ is proportional to the third order electric field susceptibility $\chi^{(3)}$ which in turn is proportional to the Kerr coefficient $n_2$. It is well known that for a Kerr type medium the index of refraction is given by $n = n_0 + n_2 |E|^2$, where $n_0$ is the linear index of refraction and $n_2$ is called the Kerr coefficient. When the latter has a positive sign the medium has self-focusing properties whereas when it is negative the medium is self-defocusing.

1.5. A generalized DNLS and nonlinear electrical lattices

Following the work of Marquié, Bilbault and Remoissenet on the nonlinear discrete electrical lattice, we will show that the dynamics of modulated waves can be modeled approximately through a generalized discrete nonlinear Schrödinger equation interpolating between the Ablowitz–Ladik equation and the DNLS [23].

We consider a lossless nonlinear electrical lattice of $N$ identical cells as shown in Fig. 2. In each of the cells there is a linear inductance $L_2$ in parallel with a nonlinear capacitor $C(V_n)$ and neighboring cells are bridged via series linear inductances $L_1$. Using Kirchhoff’s laws one derives

Fig. 2. A schematic representation of the electric network (after [23]).
a system of nonlinear discrete equations containing the nonlinear electrical charge $Q_n(t)$ of the $n$th cell and the corresponding voltage $V_n(t)$:

$$\frac{d^2 Q_n}{dt^2} = (1/L_1)(V_{n+1} + V_{n-1} - 2V_n) - (1/L_2)V_n, \; n = 1, 2, \ldots.$$  \hspace{1cm} (19)

We assume further for the charge a voltage dependence similar to that of an electrical Toda lattice [24,25]

$$Q_n(t) = AC_0 \ln[1 + V_n/A],$$  \hspace{1cm} (20)

which is justified if the inverse of the nonlinear capacitance follows a linear relation [26] according to

$$1/C(V_n) = (A + V_n)/AC_0.$$  \hspace{1cm} (21)

With the help of Eq. (19) one obtains the linear dispersion relation typical for a bandpass filter

$$\omega^2 = \omega_0^2 + 4u_0^2 \sin^2(k/2),$$  \hspace{1cm} (22)

where $\omega_0^2 = 1/L_2 C_0$ and $u_0^2 = 1/L_1 C_0$. Due to the lattice discreteness the spectrum is bounded from above by a cutoff frequency $f_{\text{max}} = \omega_{\text{max}}/2\pi = (\omega_0^2 + 4u_0^2)^{1/2}$.

Inserting the expression for $Q_n$ of Eq. (20) into Eq. (19) one obtains [23]

$$(A + V_n)\frac{d^2 V_n}{dt^2} - \left[\frac{dV_n}{dt}\right]^2 = \frac{u_0^2}{A}(A + V_n)^2\left[V_{n+1} + V_{n-1} - \left(2 + \frac{\omega_0^2}{u_0^2}\right)V_n\right].$$  \hspace{1cm} (23)

Discreteness of the lattice is maintained for a gap angular frequency $\omega_0$ much larger than any other frequency of the system, i.e. $\omega_0^2 \gg 4u_0^2$. Using this fact, we can neglect all the harmonics of a wave with any frequency $f$ since they lie above the cutoff frequency. Therefore the study is restricted to slow temporal variations of the wave envelope and solutions of the form

$$V_n(t) = \varepsilon \Psi_n(T) \exp(-i\omega t) + \varepsilon \Psi_n^*(T) \exp(+i\omega t),$$  \hspace{1cm} (24)

are searched for and $\varepsilon$ is a small parameter rescaling the time unit as $T = \varepsilon^2 t$. Upon substituting this expression in Eq. (23) and retaining only terms of order $\varepsilon^2$ we arrive at

$$2\omega_0^2/\varepsilon^2 |\Psi_n|^2 \Psi_n = - \left[g_{\Psi} \Psi_{n+1} + g_{\Psi} \Psi_{n-1} - \left(2 + \frac{\omega_0^2}{u_0^2}\right)\Psi_n\right]|\Psi_n|^2 - \left[g_{\Psi}^* \Psi_{n+1}^* + g_{\Psi}^* \Psi_{n-1}^* - \left(2 + \frac{\omega_0^2}{u_0^2}\right)\Psi_n^*\right]|\Psi_n^*|^2.$$  \hspace{1cm} (25)

Collecting now terms in $\exp(-i\omega t)$, setting $\tau = u_0^2 T/2\omega$ and $\Psi_n = \Phi_n \exp[i\tau(\omega^2 - \omega_0^2 - 2u_0^2)/u_0^2]$ gives finally

$$\frac{1}{\tau} \frac{d\Phi_n}{d\tau} + \left[\mu \Phi_{n+1} + \Phi_{n-1}\right] + \left[\mu(\Phi_{n+1} + \Phi_{n-1}) - 2v\Phi_n\right]|\Phi_n|^2 = 0,$$  \hspace{1cm} (26)

with parameters

$$\mu = \frac{1}{A^2}, \quad \nu = \frac{2\omega^2 + \omega_0^2 + 2u_0^2}{2u_0^2 A^2}.$$  \hspace{1cm} (27)
With the help of the generalized discrete nonlinear Schrödinger equation Remoissenet et al. demonstrated theoretically the possibility for the system to exhibit modulational instability leading to a self-induced modulation of an input plane wave with the subsequent generation of localized pulses. In this way energy localization in a homogeneous nonlinear system is possible and is manifested in the formation of envelope solitons [26]. Experimentally these results are confirmed by the observation of a staggered localized mode in the real electrical network.

1.6. Connection with the Holstein model

We saw previously how the nonlinear nonlocal term of the AL-DNLS equation arises in the context of the electrical lattice. Given the connection of DNLS with the Holstein model, it makes sense to ask whether this nonlocal term could be also associated with that model as well in some form. It is customary to view the nonlinear term in the pure DNLS equation as being associated with a local energy distortion that arises variationally from the adiabatic elimination of vibrational degrees of freedom. The AL equation, on the other hand, does not carry a similar physical interpretation in this context. We can, however, identify the physics behind the interpolating AL-DNLS equation in a more precise way, starting from an extension of the one-electron Holstein Hamiltonian. We assume that an electron is moving in a one dimensional tight-binding lattice with nearest neighbor matrix elements while at the same time interacts with local Einstein oscillators of mass $M$ and frequency $\omega_E$. The oscillators modulate both the local electron energies (as in the conventional Holstein model) but also affect the transfer rates; we assume that the modification of the rate between adjacent sites is determined through the average local oscillator distortion. We have the following Hamiltonian:

$$H_H = \frac{1}{2}M \sum_n (y_n^2 + \omega_E^2 y_n^2) - J \sum_n (a_n^+ a_{n+1} + a_{n+1}^+ a_n)$$

$$- \alpha \sum_n y_n a_n^+ a_m - \beta \sum_n (y_{n+1} + y_n)(a_{n+1}^+ a_n + a_n^+ a_{n+1}),$$

where $a_n^+$, $a_n$ are the electron creation and annihilation operators at site $n$ respectively, $y_n$ is the displacement of the local Einstein oscillator in the same site and $\alpha$, $\beta$ are coupling parameters. We note the physical significance of the additional interaction contribution that are proportional to $\beta$: the two terms proportional to $y_{n+1} a_{n+1}^+ a_n + y_n a_n^+ a_{n+1}$ correspond to the modulation of the transfer rate as a result of the distortion in the “destination site” whereas the other two terms depend on the distortion in the originating site.

We proceed now and perform the same adiabatic elimination of the vibrational degrees of freedom as in Section 1.3. After some straightforward manipulations and keeping only terms proportional to $\alpha^2$, $\alpha \beta$ but not of the order of $\beta^2$ results in the following stationary equation for the energy $E$:

$$E a_m = (a_{m+1}^+ + a_{m-1}^+ - \gamma |a_m|^2 a_m + \mu (a_{m+1}^+ + a_{m-1}^+)|a_m|^2 + O(\alpha \beta) + O(\beta^2) + \cdots,$$

where we set $J = -1, \gamma = \alpha^2/(M\omega_E), \mu = 2\alpha \beta/(M\omega_E)$ and we designated with $O(\alpha \beta)$ the terms $O(\alpha \beta) = \mu[(a_{m+1}^+ + a_{m-1}^+)|a_m| + |a_{m+1}^+|^2 a_{m+1}^+ + |a_{m-1}^+|^2 a_{m-1}^+].$ These last terms that are also of order $\mu$ are the modification to the transfer rate due to the local deformation in the originating site.
Clearly, if these terms are absent, the resulting equation becomes the stationary equivalent of the AL-DNLS equation. Consequently, the physical significance of the AL-type terms becomes transparent: they correspond to the modification in the transfer rates when the local distortion is taken only partially into account and depends only on the modification at the landing site. Furthermore, since dropping the terms $O(xβ)$ is equivalent to dropping two of the interaction terms (out of the four), the resulting nonhermitianity of the problem is manifested in the existence of a norm which is different from the usual probability norm of DNLS. It is easy to check that if all four terms are kept, the resulting nonlinear equation has a probability norm.

1.7. General properties of nonlinear maps

The study of the stationary properties of DNLS-like equations will be done through the use of two dimensional nonlinear maps. By now there exists a vast literature on maps (see e.g. [27—31]). We restrict ourselves to give a brief overview and summarize the basic features of such maps necessary for an analysis of the physical properties of the underlying nonlinear lattices once they have been casted into discrete maps. Nonlinear maps are used in a variety of properties ranging from stability studies of colliding particle beams in storage rings [32—35], to Anderson localization [36—39] and commensurate—incremnsurate structure studies in solid state physics [40—42].

A map $T$ of the plane generates a sequence of points $x_n = (x_n, y_n) \in \mathbb{R}^2, n = 0, 1, 2, \ldots$ by assigning to each point $x_n$ of the plane a new point via $x_{n+1} = T(x_n)$. The entire sequence $x_n$ with $n = 0, 1, 2, \ldots$ is called an orbit. The map $T$ is said to be area-preserving if for any given measurable subset $V$ of the plane, $T^{-1}(V)$ has the same area as $V$. This condition becomes equivalent to that the determinant of the Jacobian is one, i.e.

$$\text{Det}(DT) = 1,$$

for all $x$ and $D$ is the differential operator $(\partial/\partial x, \partial/\partial y)$.

We begin the discussion of the motion on the map plane with an important class of orbits, namely periodic orbits. An orbit is periodic with period $q$ if

$$x_q = x_0 + p, \quad y_q = y_0,$$

for some integer $p$. We denote such an orbit by $(p,q)$. For area-preserving maps we distinguish three types of periodic orbits depending on the stability properties of points in their neighborhood, viz. elliptic, hyperbolic (regular saddle), and reflection hyperbolic (flip saddle). The stability is determined by the eigenvalues of the tangent map. Mapping a linearized periodic orbit through its whole period in tangent space is achieved by the product of the local Jacobians taken at each periodic point

$$(DT)^q(x_0) = \prod_{n=0}^{q-1} DT(x_n).$$

Since the determinant of each local Jacobian $DT(x_n)$ is one the determinant of any product of them is also one. This implies that the eigenvalues $\lambda$ of $(DT)^q$ are either conjugate points on the unit circle or appear as real reciprocal numbers $\lambda, 1/\lambda$. The eigenvalues are connected with the trace of the
tangent map \((DT)^q\) via

\[
\lambda = \frac{1}{2} \left[ \text{Tr}(DT)^q \pm \sqrt{\left( \text{Tr}(DT)^q \right)^2 - 4} \right].
\]

The stability condition becomes thus \(|\text{Tr}(DT)^q| < 2\). But a stability classification is most conveniently given in terms of Greene’s residue [43]:

\[
R = \frac{1}{4} \left[ 2 - \text{Tr}(DT)^q \right].
\]

We summarize the results as follows [31]:

<table>
<thead>
<tr>
<th>Stability</th>
<th>\lambda</th>
<th>\text{Tr}(DT)^q</th>
<th>R</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elliptic</td>
<td>\exp(2\pi i\omega)</td>
<td>((-2, 2))</td>
<td>((0, 1))</td>
</tr>
<tr>
<td>Hyperbolic</td>
<td>&gt; 0</td>
<td>&gt; 2</td>
<td>&lt; 0</td>
</tr>
<tr>
<td>Reflection</td>
<td>Hyperbolic</td>
<td>&lt; 0</td>
<td>&lt; -2</td>
</tr>
</tbody>
</table>

Nearby points of each elliptic periodic point rotate about the point in ellipses by an angular increment \(\arccos[1 - 2R]\) on average per iteration of the map \((DT)^q\). Equivalently the rotation frequency \(\omega\) is linked with the value of the residue via \(R = \sin^2(\pi \omega)\). For irrational \(\omega\) the orbit never returns to its initial point and such an orbit is called quasiperiodic. The orbit points come to lie on invariant closed curves. According to the Kolmogorov–Arnold–Moser (KAM) theorem the orbit is stable provided \(R \neq 0, 3/4, 1/2\). For the cases of \(R = 0, 3/4, 1/2\) corresponding to the so-called Arnold resonances the linearization does not suffice for a stability analysis [44].

For \(R < 0\), where the points of the periodic orbit are hyperbolic, nearby points diverge from them with an exponential separation rate \(|1 - 2R + 2\sqrt{R^2 - R}|\).

Upon varying a parameter of the map the location of the periodic orbit as well as its residue will be changed. If the residue changes from a positive value to the negative range then a tangent bifurcation takes place where an elliptic point handles its stability over to a hyperbolic point. Whenever the residue passes the value of one from below (if \(\omega = 1/2\)) a stable elliptic orbit converts into an unstable hyperbolic point with reflection accompanied by the creation of two new stable elliptic points via a period-doubling bifurcation. The latter remain stable until the corresponding value of \(\omega\) reaches one half and another period doubling bifurcation occurs destroying also the nearby quasiperiodic orbits. After a cascade of such period doubling bifurcations local chaos appears. The character of motions on the map depends on the initial conditions. In general we distinguish regular (integrable) and irregular (chaotic) regimes for a map. A map is said to be integrable in the Liouville sense if there exists a sufficient number of integrals. An integral is a function on the map-plane \(I(x)\), which is invariant under the map, that is \(T(I(x)) = I(x)\). More precisely, if a \(2N\)-dimensional map possesses \(N\) independent integrals \(I_j, j = 1, 2, \ldots, N\) which are in involution, i.e. all the mutual Poisson brackets vanishes \(\{I_n, I_m\} = 0\), then the motion is integrable and lies on a family of \(N\)-dimensional nested tori appearing in the case of \(N = 2\) as closed invariant curves.
We discuss now the transition from regular behavior to the occurrence of global chaos in a two-dimensional area-preserving map. Applying a small nonintegrable perturbation to an integrable map the KAM theorem assures the survival of most of the invariant tori for sufficiently weak perturbations. However, some of the invariant tori, namely those with rotational frequency \( \omega \) close enough to a rational value, will break up into resonance chains (Poincaré–Birkhoff-chains). These resonance chains consist of periodic points of alternating stability type. The elliptic points are again surrounded by stable quasiperiodic cycles. The stable and unstable manifolds belonging to the unstable hyperbolic points embrace the stability zones around the elliptic points and an island like structures are formed called resonances. In the vicinity of the hyperbolic points local stochasticity (chaos) occurs due to the tangling of the invariant stable and unstable manifolds.

With further increase in the perturbation strength the width of the resonance islands grows and the resonant cycles break up giving birth to new resonance chains of higher order while the other quasiperiodic cycles remain stable due to the KAM theorem. We find local regions of regular and irregular motions coexisting on the map plane exhibiting a complicated hierarchical structure of islands within islands. At the same time with increased island width KAM cycles lying in between two neighboring resonances can be destroyed as a result of resonance overlap. When further increasing the nonintegrability parameter a very complicated network of orbits develops where more and more regions are covered by chaotic orbits. Finally, above a critical perturbation strength even the most resisting final KAM cycle breaks up and the phase plane will be densely covered with global chaos except for a few tiny islands of stability.

There exists a useful property for a special class of area-preserving maps. If the map \( T \) factors according to \( T = T_1 T_2 \), with \( T_1 \) and \( T_2 \) being orientation-reversing involutions, i.e. they satisfy

\[
T_1^2 = T_2^2 = 1, \quad \det(DT_1) = \det(DT_2) = -1,
\]

then \( T^{-1} = T_2 T_1 \). That the map \( T \) can be written as the product of two orientation-reversing involutions establishes its reversibility. The invariant sets of the two involutions form the symmetry lines of the map. For reversible area-preserving maps there exists a particular symmetry line on which at least one point of every positive residue Poincaré–Birkhoff orbit (elliptic or reflection hyperbolic) lays. This line is called the dominant symmetry line. For reversible area-preserving maps it suffices therefore a one-dimensional search for the periodic orbits. Furthermore one can prove that the homoclinic orbits belonging to the (transversal) intersections of the stable and unstable manifolds of a hyperbolic point fall on symmetry lines in reversible area-preserving maps [45]. The next section is devoted to integrable maps since they are of importance both for the study of soliton equations as well as serve as the starting point for perturbation theory (see e.g. [46]).

1.8. Integrable mappings and soliton equations

We review the properties of nonlinear integrable maps describing the solution behavior of certain kinds of (stationary) solutions of nonlinear integrable lattices. Integrable partial difference equations or nonlinear integrable lattices may arise from space discretization of integrable nonlinear partial differential equations giving differential-difference (\( D \Delta \)) equations. The latter give rise to hierarchies of integrable PDEs [47] and are of importance especially from the point of view of integrability in classical nonlinear Hamiltonian systems in general. Many physical systems are close to integrable systems so that their study is also of practical interest to follow e.g. bifurcations.
and the transition to chaos with a perturbational approach [48]. Furthermore, nonlinear integrable maps are also of interest for the construction of numerical integration schemes of nonlinear PDE’s [49,50].

The oldest example of a nonlinear integrable map is certainly Jacobi’s celebrated elliptic billiard [51]. Quispel et al. [52,53] reported on an eighteen-parameter family of nonlinear integrable maps which is actually a generalization of the four-parameter family found by McMillan [54]. The authors established a linkage of these maps to soliton theory and statistical mechanics. They treated in detail various examples of physical interest, namely the stationary reductions of a $DA$ isotropic Heisenberg spin chain, and besides the discrete modified Korteweg–de Vries equation, and the integrable $DA$ nonlinear Schrödinger equation, viz. the Ablowitz–Ladik equation. All of these stationary soliton equations are described by symmetric integrable maps. We summarize here their results for the discrete modified Ablowitz–Ladik equation ($V = 1$):

$$
\frac{d\psi_n}{dt} = \psi_{n+1} + \psi_{n-1} + \mu |\psi_n|^2 [\psi_{n+1} + \psi_{n-1}] . \tag{36}
$$

The stationary solutions follow from the ansatz $\psi_n = \phi_n \exp(-i\omega t)$ with real $\phi_n$, yielding a two-dimensional map

$$
\omega \phi_n - (1 + \phi_n^2)[\phi_{n+1} + \phi_{n-1}] = 0 . \tag{37}
$$

This map was studied by Ross and Thompson [55]. The map possesses the following integral of motion

$$
\omega \phi_{n+1} \phi_n - (1 + \mu \phi_n^2)\phi_{n+1}^2 \phi_n^2 = K , \tag{38}
$$

where $K$ is the integration constant. Particularly for $K = 0$ we obtain the separatrix solution corresponding to the stationary AL-soliton

$$
\phi_n = \sinh \beta \sinh[\beta(n - x_0)] , \tag{39}
$$

where $\beta$ is a parameter and $x_0$ specifies the soliton center.

Since this map can be written as the product of two involutions it is a reversible map. It turns out to be a special case of the eighteen-parameter family of integrable reversible planar maps given by

$$
\phi_{n+1} = \frac{f_1(\phi_n) - \phi_{n-1} f_2(\phi_n)}{f_2(\phi_n) - \phi_{n-1} f_3(\phi_n)} , \tag{40}
$$

where

$$
f(\Phi) = (M_0 \Phi) \times (M_1 \Phi) , \tag{41}
$$

with $\Phi = (\phi^2, \phi, 1)^T$ and

$$
M_n = \begin{pmatrix}
\alpha_n & \beta_n & \gamma_n \\
\delta_n & \varepsilon_n & \zeta_n \\
\kappa_n & \lambda_n & \mu_n
\end{pmatrix} , \quad n = 0, 1 . \tag{42}
$$
Each member of this family possesses a one-parameter family of invariant curves fulfilling the relation
\[
(x_0 + Kx_1)\phi_{n+1}^2 + (\beta_0 + Kb_1)(\phi_{n+1}^2 + \phi_n^2) + (\gamma_0 + K\gamma_1)\phi_{n+1}^2 + \phi_n^2 + (\epsilon_0 + Ke_1)\phi_{n+1} + (\zeta_0 + K\zeta_1)(\phi_{n+1} + \phi_n) + (\mu_0 + K\mu_1) = 0.
\] (43)
A parameterization of this equation in terms of Jacobian elliptic functions is possible and in dependence of the integration constant periodic, quasiperiodic as well as solitonic solution behavior can be distinguished.

There exist many more examples for differential-difference equations (D\AE) the stationary solutions of which are determined by a map of the type of (40)–(43). This led Quispel et al. to the following conjecture: “Consider a differential-difference equation. Then every autonomous difference equation obtained by an exact reduction of the D\AE is an integrable mapping”. However one should be aware that the reverse of this conjecture does not necessarily hold [52]. On the other hand, for many physically relevant problems the solutions cannot be given at all in closed analytical form and rather irregular (chaotic) dynamics is encountered pointing to nonintegrability as it is the case also for DNLS.

2. Spatial properties of integrable and nonintegrable discrete nonlinear Schrödinger equations

2.1. Integrable and nonintegrable discrete nonlinear Schrödinger equations

The nonlinear Schrödinger equation (NLS) is one of the prototypical nonlinear partial differential equations, the study of which has lead to fundamental advances in nonlinear dynamics. The study of NLS was motivated by a large number of physical and mathematical problems ranging from optical pulse propagation in nonlinear fibers to hydrodynamics, condensed matter physics and biophysics. We now know that NLS provides one of the few examples of completely integrable nonlinear partial differential equations [56]. Since most work in nonlinear wave propagation involves at some stage a numerical study of the problem, the issue of the discretization of NLS was addressed early in Ref. [56]. Ablowitz and Ladik noticed that among a large number of possible discretizations of NLS there is one that is also integrable [16]. The study of the integrable version of the discrete nonlinear Schrödinger equation, called hereafter Ablowitz–Ladik, or AL equation, showed that it has solutions which are essentially the discrete versions of the NLS solitons [16]. Another discrete version of the NLS equation was studied in detail later [1]; the latter usually referred to as discrete nonlinear Schrödinger equation DNLS or discrete self-trapping equation (DST), has quite a number of interesting properties, but it is not integrable [50]. We note that the motivation for studying the two discrete versions of NLS, viz., the AL equation and the DNLS equation respectively, are quite different: The AL equation, on one hand, has very interesting mathematical properties, but not very clear physical significance; the introduction of the DNLS equation, on the other hand, is primarily motivated physically. In particular, the latter seems to arise naturally in the context of energy localization in discrete condensed matter and biological systems as well as in optical devices [1–7,57–67]. Even though in these problems one typically assumes that the length scale of the nonlinear wave is much larger than the lattice spacing and therefore NLS provides a good description for those problems, the study of DNLS (and AL)
The equation is important when the size of the physical system is small or the nonlinear wave is strongly localized.

The motivation for the present chapter is an equation introduced by Salerno [17] and studied recently by Cai et al. [18] that interpolates between DNLS and AL equations while containing these two as its limits [17]. By varying the two nonlinearity parameters of this new equation one is able to monitor how “close” it is to the integrable or nonintegrable version of the NLS. The new equation finds its physical explanation in the context of the nonlinear coupler problem [68] and the application in a nonlinear electrical transmission line [23]. However, its basic merit is that it allows us to study the interplay of the integrable and nonintegrable NLS-type terms in discrete lattices. In addition, one can address the issue of “nonlinear eigenstates” of the new equation and their connection to the integrability/nonintegrability issue.

Before presenting the basic properties of the stationary (generalized) DNLS we give a review of other papers on it: Salerno [17] studied the quantum deformation of AL-DNLS and derived for the two-particle chain (a dimer) some explicit formulas for the first excited levels of the quantized version showing that they can be continuously deformed into the corresponding ones of the two extreme limits of $\gamma = 0$ respectively $\mu = 0$. Kivshar and Peyrard obtained the DNLS in their study of modulational instability in the discrete nonlinear Klein–Gordon lattice [69]. The DNLS arises there as the envelope function in a rotating wave approximation for slowly modulated carrier waves of the Klein–Gordon field amplitudes. Furthermore, for comparison they studied also the AL equation. Claude et al. investigated the creation and stability of localized modes in Fermi–Pasta–Ulam chains and nonlinear discrete Klein–Gordon lattices [70]. Their ansatz function for localized modes resulted in the DNLS. For a perturbational approach they wrote DNLS as a perturbed AL system yielding the AL-DNLS equation. Cai et al. studied the AL-DNLS equation focusing interest on the interplay of integrability and nonintegrability [18]. They pointed out that the localized states of the AL system are the AL-solitons. Furthermore they showed that for AL-DNLS there exist two types of localized modes. One type is a state with in-phase oscillations of neighboring particles having oscillation frequencies lying below the linear phonon band and is called an unstaggered state. The other one exhibits out-of-phase oscillations of neighboring particles and has oscillation frequencies above the linear (phonon) band and is called a staggered state. For further discussion of localized (stationary) states in DNLS we refer to Section 3. Kivshar and Salerno studied analytically and numerically modulational instability for the AL-DNLS with emphasis on how different discretizations of the nonlinear interaction term change modulational instability in the lattice [71]. Hays et al. studied a generalized lattice with equation $i\dot{A}_j + F(|A|^2)(A_{j+1} + A_{j-1}) + F(|A|^2)A_j = 0$ that contains DNLS, AL and several other models as special cases. They developed a fully nonlinear modulation theory for harmonic plane wave solutions of the form $A_n(t) = a \exp[\imath(\kappa n - \omega t)]$ [72]. Konotop et al. [73] and Cai et al. [74] proved integrability of the dynamics of the AL system in a time-varying, spatially uniform electric field along the chain direction which is of the form $V_n = \delta(t) n$. In the limit of a static electric field, the system exhibits a periodic evolution which is a nonlinear counterpart of Bloch oscillations. Further it was shown that for certain strengths of a harmonic field dynamical localization can be caused which can be interpreted as a parametric resonance effect. (We refer also to Section 4.7 for a treatment of similar effects in Kronig–Penney models.) Cai et al. extended the (integrable) AL system study by incorporating the integrability-breaking DNLS term as well and showed that Bloch oscillations and dynamical localization are maintained in the AL-DNLS system. Hence they
are effects of the lattice and does not depend on integrability. The special case of a AL system with a potential depending linearly on the spatial coordinate, i.e. \( V_n = A n \), was treated Scharf and Bishop by means of the inverse scattering transform. These authors obtained a UV pair proving integrability of the model [75]. Hennig et al. investigated the formation of breatherlike impurity modes in a “disordered” version of the AL-DNLS containing a single impurity [76]. An interesting study on soliton interactions and beam steering in nonlinear waveguide arrays modeled by DNLS was performed by Aceves and co-workers in Refs. [77–79]. Special attention is paid to the existence and control of the propagation of stable localized wave packets in waveguide arrays. It is shown that localized modes with energy stored only in a few lattice sites are the preferred stable steady patterns of the system. Among several analytical methods (discrete variational approaches) also soliton perturbation theory based on a perturbed AL system was used. The issue of perturbation theory of discrete nonlinear Schrödinger equations was also addressed in [80].

2.2. The generalized nonlinear discrete Schrödinger equation

The main purpose of this section is to study the stationary properties of the following generalized discrete nonlinear Schrödinger equation (GDNLS)

\[
\frac{i\,d\psi_n(t)}{dt} = (V + \mu|\psi_n(t)|^2)[\psi_{n+1}(t) + \psi_{n-1}(t)] - \gamma|\psi_n(t)|^2\psi_n(t),
\]

where \( \psi_n \) is a complex amplitude, \( \mu \) and \( \gamma \) are nonlinearity parameters and \( V \) is the transfer matrix element coupling adjacent oscillators at site \( n \) and \( n \pm 1 \), respectively. We note that Eq. (44) interpolates between two possible discretizations of NLS viz. the DNLS and AL equation obtained by setting \( \mu = 0 \) (with \( \gamma \neq 0 \)) and \( \gamma = 0 \) (with \( \mu \neq 0 \)), respectively [17]. To reduce the number of parameters we use a time scaling according to \( V t \to t \) and introduce the ratios \( \tilde{\gamma} = \gamma/V \) and \( \tilde{\mu} = \mu/V \). For ease of notations we drop the tildes afterwards. We remark that a linear contribution \( \epsilon_n \psi_n(t) \) appearing on the right hand side (r.h.s.) of the Eq. (44) can be removed by a global phase transformation \( \psi_n(t) \to \exp(-i\epsilon t)\psi_n(t) \).

The stationary equation is obtained by substituting \( \psi_n(t) = \phi_n \exp(-iEt) \) in Eq. (44) giving

\[
E\phi_n - (1 + \mu|\phi_n|^2)[\phi_{n+1} + \phi_{n-1}] + \gamma|\phi_n|^2\phi_n = 0,
\]

with complex variables \( \phi_n \) and \( E \) is the phase of the stationary ansatz. The stationary equation (45) was analyzed in the aforementioned extreme limits through map approaches in Refs. [52,81,82]. The stationary real-valued AL system satisfies an integrable mapping which is contained in the 18-parameter family of integrable mappings of the plane reported by Quispel et al. in [53]. In this section we will present an analysis of Eq. (45) and discuss the interplay of the integrable and nonintegrable nonlinear terms in the context of the complete equation [83].

Eq. (45) may be rewritten as

\[
\phi_{n+1} + \phi_{n-1} = \frac{E + \gamma|\phi_n|^2}{1 + \mu|\phi_n|^2}\phi_n,
\]

which obviously reduces to a degenerate linear map if \( \gamma = E\mu \). Although reduction of the complex-valued amplitude dynamics to a two-dimensional real-valued map is possible, (see Section 2.4), we concentrate in this section on the study of the recurrence relation \( \phi_{n+1} = \phi_n + (\phi_n \phi_{n-1}) \) appropriate for the investigation of stability of the nonlinear lattice chain. Eq. (46) can also be derived as the
relation which makes the action functional
\[
F = \sum_n \left\{ \frac{1}{\mu} \left( E - \frac{\gamma}{\mu} \right) \ln(1 + \mu|\phi_n|^2) + \frac{\gamma}{\mu} |\phi_n|^2 - (\phi_n^* \phi_{n+1} + \phi_n \phi_{n+1}^*) \right\}
\]
(47)
an extremum. In the limit \( \mu = 0 \), the latter is replaced by
\[
F = \sum_n \left\{ E|\phi_n|^2 + \frac{1}{2} \gamma |\phi_n|^4 - (\phi_n^* \phi_{n+1} + \phi_n \phi_{n+1}^*) \right\}.
\]
(48)
The extremal sets \( \{\phi_n\} \) define the orbits and together with appropriate boundary conditions determine the solutions of a particular physical problem. However, concerning the stability properties one has to distinguish between the (dynamical) stability of the physical solutions and the (linear mapping) stability of the corresponding map orbit generated by the recurrence relation
\[
\phi_{n+1} = \phi_{n+1}(\phi_n, \phi_{n-1}) \quad [41,42].
\]
In general, a dynamical stable solution minimizing the action corresponds to a linearly unstable map orbit, whereas physically unstable solutions corresponding to maximum energy configurations are reflected in the map dynamics as linearly stable orbits. In the present study we focus on the transmission properties of the "nonlinear lattice" of Eq. (45), since finding the linearly stable map solutions (propagating wave solutions) is essential.

2.3. Stability and regular solutions

The second-order difference equation (46) can be regarded as a symplectic nonlinear transformation relating the amplitudes in adjacent lattice sites. This transformation can be considered as a dynamical system where the lattice index \( n \) plays the role of the discrete time \( n \). The resulting dynamics of the two-component (amplitude) vector \((\phi_{n+1}, \phi_n)^T\) is determined by the following Poincaré map:
\[
\mathcal{M}_n: \begin{pmatrix} \phi_{n+1} \\ \phi_n \end{pmatrix} = \begin{bmatrix} E_n & -1 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} \phi_n \\ \phi_{n-1} \end{pmatrix},
\]
(49)
where the nonlinear transfer matrix depends on the amplitude \( \phi_n \) through
\[
E_n = \frac{E + \gamma |\phi_n|^2}{1 + \mu |\phi_n|^2}.
\]
(50)
The stability of the orbits \( \{\phi_n\}, (n = 0, \ldots, N) \), or equivalently the transmission properties of the nonlinear lattice of chain length \( N \), is governed by the solution behavior of the corresponding linearized equations in the neighborhood of an orbit ranging from \((\phi_0, \phi_1)\) to \((\phi_{N-1}, \phi_N)\). For a semi-infinite (or infinite) one-dimensional lattice chain the (finite) sequence \( \{\phi_n\}, (n = 0, \ldots, N) \), defines an orbit segment.

To investigate the linear stability of a given orbit we introduce a small (complex-valued) perturbation \( u_n \) and consider the perturbed orbit \( \phi_n \to \phi_n + u_n \). Linearizing the map equations results in the second-order difference equation for the perturbations \( u_n \):
\[
u_{n+1} + u_{n-1} = \frac{1}{(1 + \mu |\phi_n|^2)^2} \{ (E + 2 \gamma |\phi_n|^2 + \mu \gamma |\phi_n|^4) u_n + (\gamma - E \mu) \phi_n^2 u_n^* \}.
\]
(51)
Writing further \( \phi_n = A_n + iB_n \) and \( u_n = x_n + iy_n \) with real \( A_n, B_n, x_n, y_n \), we obtain the four-dimensional map in tangent space
\[
\begin{pmatrix}
  x_{n+1} \\
  y_{n+1}
\end{pmatrix} =
\begin{pmatrix}
  E_n^x & -1 & \beta & 0 \\
  1 & 0 & 0 & 0 \\
  \beta & 0 & E_n^y & -1 \\
  0 & 0 & 1 & 0
\end{pmatrix}
\begin{pmatrix}
  x_n \\
  y_n \\
  x_{n-1} \\
  y_{n-1}
\end{pmatrix}
\equiv J_n
\begin{pmatrix}
  x_n \\
  y_n \\
  x_{n-1} \\
  y_{n-1}
\end{pmatrix}
\] (52)

with
\[
E_n^x = \frac{1}{[1 + \mu(A_n^2 + B_n^2)]^2}[E + E\mu(B_n^2 - A_n^2) + \gamma(3A_n^2 + B_n^2) + \mu\gamma(A_n^2 + B_n^2)^2] ,
\] (53)
\[
E_n^y = \frac{1}{[1 + \mu(A_n^2 + B_n^2)]^2}[E + E\mu(A_n^2 - B_n^2) + \gamma(3B_n^2 + A_n^2) + \mu\gamma(A_n^2 + B_n^2)^2] ,
\] (54)
\[
\beta = \frac{2}{[1 + \mu(A_n^2 + B_n^2)]^2}(\gamma - E\mu)A_nB_n .
\] (55)

First we deal with a local stability criterion. The eigenvalues \( \tilde{\alpha} \) of the Jacobian matrix \( J_n \) follow from the characteristic polynomial given by
\[
\tilde{\alpha}^4 - \frac{2}{[1 + \mu|\phi_n|^2]^2}[E + 2\gamma|\phi_n|^2 + \mu\gamma|\phi_n|^4](1 + \tilde{\alpha}^2)\tilde{\alpha}
+ \left[ 2 + \frac{1}{[1 + \mu|\phi_n|^2]^2} \right] \left( E^2 + 4\gamma E|\phi_n|^2 + (4\gamma E - 3\gamma^2 - \mu^2 E^2)|\phi_n|^4
+ 4\gamma^2 \mu|\phi_n|^6 + \gamma^2 \mu^2 |\phi_n|^{8} \right) \tilde{\alpha}^2 + 1 = 0 .
\] (56)

Being interested in the derivation of a sufficient condition for linear stability we note that if the following inequality holds
\[
E\mu \geq \gamma ,
\] (57)
and if additionally \( |E| < 2 \) then all four eigenvalues \( \tilde{\alpha} \) lie on the unit circle. On the other hand, for the following (eigenvalue) equation
\[
\tilde{\alpha}^4 - \frac{2}{[1 + \mu|\phi_n|^2]^2}[E + 2\gamma|\phi_n|^2 + \mu\gamma|\phi_n|^4](1 + \tilde{\alpha}^2)\tilde{\alpha}
+ \left[ 2 + \frac{1}{[1 + \mu|\phi_n|^2]^2} \right] \left( E^2 + 2\gamma E|\phi_n|^2 + \mu\gamma|\phi_n|^4 \right) \tilde{\alpha}^2 + 1
\equiv \left( \tilde{\alpha}^2 - \frac{1}{[1 + \mu|\phi_n|^2]^2}[E + 2\gamma|\phi_n|^2 + \mu\gamma|\phi_n|^4] \tilde{\alpha} + 1 \right)^2 = 0 ,
\] (58)
can be readily shown that whenever the inequality (57) holds then the Eq. (58) has only complex solutions of modulus one. Moreover, for fixed parameters \( E, \gamma \) and \( \mu \) we find that \( |\text{Im}(\tilde{\alpha})| \geq |\text{Im}(\alpha)| \).
We conclude that as long as the system (58) possesses exclusively complex roots so does the original Eq. (56). The characteristic polynomial (58) can be related to the (original) eigenvalue problem of Eqs. (51)—(56) if we introduce in (51) polar coordinates $\phi_n = r_n \exp(i\theta)$ and neglect rapidly oscillating terms of the order $\phi_n^2 \sim r_n^2 \exp(2i\theta)$. The corresponding map in tangent space reads then as

$$
\begin{pmatrix}
  x_{n+1} \\
  x_n \\
  y_{n+1} \\
  y_n
\end{pmatrix}
= 
J(\mathcal{M}_n)
\begin{pmatrix}
  x_n \\
  x_{n-1} \\
  y_n \\
  y_{n-1}
\end{pmatrix}.
$$

(59)

Hence, the original four-dimensional problem splits into two identical two-dimensional systems. Therefore it suffices to investigate the two-dimensional local variational equation assigned to Eq. (58) which is given by

$$
\begin{pmatrix}
  \delta\phi_{n+1} \\
  \delta\phi_n
\end{pmatrix} = J(\mathcal{M}_n)
\begin{pmatrix}
  \delta\phi_n \\
  \delta\phi_{n-1}
\end{pmatrix},
$$

(60)

where $J(\mathcal{M}_n) = \frac{\partial (\phi_{n+1}, \phi_n)}{\partial (\phi_n, \phi_{n-1})}$ is the real matrix

$$
J(\mathcal{M}_n) = \begin{bmatrix}
  \tilde{E}_n(\phi_n) & -1 \\
  1 & 0
\end{bmatrix},
$$

(61)

with

$$
\tilde{E}_n(\phi_n) = \frac{E + 2\gamma|\phi_n|^2 + \mu\gamma|\phi_n|^4}{1 + \mu|\phi_n|^2}.
$$

(62)

Mapping the variations from $(\delta\phi_0, \delta\phi_1)$ to $(\delta\phi_{N-1}, \delta\phi_N)$ is accomplished by the product of the real $2 \times 2$ symplectic Jacobian transfer matrices

$$
J(\mathcal{M}) = \prod_{n=1}^{N-1} J(\mathcal{M}_n).
$$

(63)

Before proceeding with the stability analysis of the nonlinear discrete Schrödinger equation (45), we note that in the corresponding linear tight-binding model given by the equation $\phi_{n+1} + \phi_{n-1} = E\phi_n$, the (stable) solutions in the passing band of $|E| < 2$ are parameterized by a wave vector $k \in [-\pi, \pi]$ corresponding to the linear dispersion relation $E = 2\cos(k)$. Upon increasing the nonlinearity parameters $\gamma$ and $\mu$ from zero, the nonlinear dispersion relation for $\phi_n = \phi_0 = \text{constant}$ reads as $E = 2\cos(k) + [2\mu \cos(k) - \gamma]|\phi_0|^2$ and the stability of the orbits can alter where rational values of the winding number $k/(2\pi) = p/q$, with integers $p, q$, yield periodic orbits whereas irrational values result in quasiperiodic orbits.

First of all, we study the linear stability of periodic orbits $\phi_{n+q} = \phi_n$ with cycle lengths $q$. The linear stability of a periodic orbit is governed by its multipliers, i.e. the eigenvalues of the corresponding linearized map. In examining the linear stability of the periodic orbits we make use of the fact that solving the linearized equations becomes equivalent to a band problem of a linear discrete Schrödinger (tight-binding) equation with periodic potential (see e.g. [84–86]) where we can invoke the (linear) transfer matrix method [87].
In the following we derive a sufficient criterion for linear stability. We substitute $\delta \phi_n \equiv \varphi_n$, and the linearized equation corresponding to (46) can be written in matrix notation

$$
\begin{pmatrix}
\varphi_{n+1} \\
\varphi_n
\end{pmatrix} = M_1(\vec{E}_n) \begin{pmatrix}
\varphi_n \\
\varphi_{n-1}
\end{pmatrix},
$$

(64)

where $M_1(\vec{E}_n) \equiv J(\varphi_n)$ and $\vec{E}_n$ are given in Eqs. (61) and (62), respectively. The matrix product

$$
M_q = \prod_{n=0}^{q-1} M_1(\vec{E}_n)
$$

(65)

transfers $(\varphi_0, \varphi_{-1})$ to $(\varphi_q, \varphi_{q-1})$ through a complete periodic cycle of length $q$. Since the periodic orbit members enter the individual transfer matrices $M_1(\vec{E}_n)$, Eq. (64) represents a linear equation with periodic potential $\vec{E}_n = \vec{E}_n(\varphi_n)$ and $\varphi_{n+q} = \exp(ikq)\varphi_n$ [88]. Thus $M_q$ has eigenvalues $\exp(\pm ikq)$, and its trace is given by

$$
\text{Tr}[M_q] = 2\cos(kq),
$$

(66)

which leads to the condition $|\text{Tr}[M_q]| \leq 2$ for the stable Bloch solutions and to two equivalence classes for the total symplectic transfer matrix $M_q$ corresponding to different stability properties. For the real matrix $M_q$ these equivalence classes are determined by the solution of the eigenvalue problem,

$$
z^2 - (\text{Tr}[M_q])z + 1 = 0,
$$

(67)

where the roots $z_{1,2}$ determine the multipliers of the periodic orbit [28]. When $|\text{Tr}[M_q]| < 2$, then $M_q$ has a pair of complex conjugate eigenvalues $z_{1,2}$ on the unit circle leading to a stable elliptic periodic cycle or an oscillating Bloch-type solution (passing band state). When $|\text{Tr}[M_q]| > 2$, this yields real reciprocal eigenvalues corresponding to an unstable hyperbolic periodic cycle which has to be excluded as physically unacceptable, since it increases exponentially with larger chain length (stop band or gap state).

Computation of $\text{Tr}[[\prod_{n=0}^{q-1} M_1(\vec{E}_n)]]$ for a general periodic orbit of arbitrary cycle length $q$ requires tedious algebra. However, if $\gamma, \mu$ and $E$ satisfy the inequality (57) then $|\vec{E}_n(\varphi_n)| < |E|$ and each individual transfer (Jacobian) matrix $M_1$ has the important property

$$
\|M_1(\vec{E}_n)\| \leq \|T_1(E_n)\|,
$$

(68)

where

$$
T_1(E_n) = \begin{bmatrix}
E_n & -1 \\
1 & 0
\end{bmatrix},
$$

(69)

is the individual transfer matrix of a linear lattice chain at constant $E_n = E$. The norm of a matrix $A$ is defined by $\|A\| = \max_{\|z\|=1} \|Az\|$, i.e. the natural norm induced by the vector norm $\|z\|$ [89]. We note that the inequality (68) imposes no restriction to the amplitudes $\varphi_n$, since it is a global feature of the mapping in the parameter range satisfying (57). For the linear lattice chain the total transfer matrix satisfies $|\text{Tr}[T_q(E)]| = |\text{Tr}[[\prod_{n=0}^{q-1} T_1(E_n)]]| < 2$ as long as $|E_n| = |E| < 2$, i.e. is in the range of the passing band. Furthermore, because all the local Jacobians are identical, it is easy to
show that the global trace $\text{Tr}[T_4(E)] = 2 \cos(\theta q)$, where $\theta = \cos^{-1}(\frac{1}{2} \text{Tr}[T_4]) = \cos^{-1}(\frac{1}{2} E)$. With the help of $\|A^n\| \leq \|A\|^n$ and the modified inequality (68)

$$\prod_{n=0}^{q-1} \{\|T_1(E_n)\| - \|M_1(\tilde{E}_n)\| \} \geq 0$$

(70)

we infer that

$$\prod_{n=0}^{q-1} \|T_1(E_n)\| \geq \prod_{n=0}^{q-1} \|M_1(\tilde{E}_n)\|.$$  

(71)

Further, a natural matrix norm satisfies the inequality

$$\max|x_{1,2}| \leq \|A\|.$$  

(72)

Using Eqs. (71) and (72), one sees that the spectral radius of the matrix $\prod_{n=0}^{q-1} [M_1(\tilde{E}_n)]$ is bounded from above by $\prod_{n=0}^{q-1} [T_1(E_n)]$. Since the eigenvalues are related to the trace via $\text{Tr}[A] = (\alpha + 1/\alpha)$, it can be readily shown that, whenever Eq. (57) holds, then $|\text{Tr}[\prod_{n=0}^{q-1} M_1(\tilde{E}_n)]| \leq |\text{Tr}[\prod_{n=0}^{q-1} T_1(E_n)]| = |2 \cos(\theta q)| < 2$. Hence, all periodic orbits for the nonlinear lattice chain are linearly stable. Moreover, since for symplectic mappings the linear stability is both necessary and sufficient for nonlinear stability [28,44,90] the existence of KAM tori close to the periodic orbits is guaranteed for the combined AL-DNLS chain, when $E \mu \geq \gamma$ and $|E| < 2$. With the help of this sufficient stability condition we show in Section 2.4 below, that the reduced two-dimensional (real-valued) map then possesses a stable period-1 orbit which is surrounded by integrable quasiperiodic solutions.

On the other hand, from the stability condition $|\text{Tr}[M_4]| < 2$ one can also deduce a necessary condition for the stability of a periodic orbit. The transfer matrix depends parametrically on $\tilde{E}_n$. Therefore, in order to be compatible with $|\text{Tr}[M_4(\tilde{E}_n)]| < 2$ we have to distinguish between allowed and forbidden $\tilde{E}_n$, if $\gamma > E \mu$. Because of $\tilde{E}_n = \tilde{E}_n(|\phi_n|)$, the allowed $\tilde{E}_n$ become amplitude dependent imposing constraints on the latter. Since each member of a periodic orbit family exhibits the same stability type [28], it is sufficient to consider only one of the periodic points of each family, e.g. $|\text{Tr} M_1(\tilde{E}_n)| < 2$. A periodic orbit point is compatible with the allowed $E$-range of the passing band when the amplitude fulfills the necessary condition:

$$|\phi_n|^2 < \frac{1}{\mu} \left( \frac{E - 2}{2 - \gamma/\mu} - 1 \right),$$

(73)

which reduces to $|\phi_n|^2 < (1 - E/2)/\gamma$ in the limit $\mu \to 0$. When the condition (73) is violated a stop band (gap) state is encountered.

Generally, whenever the inequality (57) holds, we are able to prove that all solutions of the combined AL-DNLS equation (46) are regular. The linear stability of general orbits is governed by a Lyapunov exponent (LE) representing the rate of growth of the amplitudes and is defined as [28,41,91]

$$\lambda = \lim_{N \to \infty} \lambda_N = \lim_{N \to \infty} \frac{1}{2N} \ln \left[ \prod_{n=0}^{N} J_n \right],$$

$$\equiv \lim_{N \to \infty} \frac{1}{2N} \ln \| J_N^T J_N \| = \lim_{N \to \infty} \lambda_N.$$  

(74)
An orbit is linearly stable (unstable) with respect to the initial conditions if \( \lambda = 0 \) (\( \neq 0 \)). It has been proven that almost all initial conditions (except for a set of measure zero) lead to the largest LE [92,93], which in our case is the non-negative LE \( \lambda \geq 0 \). In the parameter range \( E\mu \geq \gamma \) and \( |E| < 2 \) we get with the help of the norm properties \( \|A^n\| \leq \|A\|^n \) and \( \|AB\| \leq \|A\|\|B\| \):

\[
\lambda_N = \frac{1}{2N} \ln \|J_N^T J_N\| \leq \frac{1}{2N} \ln \left( \|J_N^T\| \|J_N\| \right) = \frac{1}{N} \ln \left( \prod_{n=0}^{N} J_n \right) \leq \frac{1}{N} \ln \left( \prod_{n=0}^{N} \|J_n\| \right),
\]

and \( J_n \) is the Jacobi matrix determined by Eq. (52). Denote by \( \|J_{\text{max}}\| = \max_n \|J_n\| \), then we get

\[
\lambda_N \leq \frac{1}{N} \ln \|J_{\text{max}}\| = \ln \|J_{\text{max}}\| = \ln \|A^{-1} A J_{\text{max}} A^{-1} A\| \leq \ln \|A^{-1}\|
\]

\[
+ \ln \|\text{diag}(\tilde{a})\| + \ln \|A\| = 0,
\]

with \( A \) being the matrix whose columns are formed by the (normalized) eigenvectors of \( J_{\text{max}} \) and \( \text{diag}(\tilde{a}) \) is the diagonal matrix the elements of which are the eigenvalues of \( J_{\text{max}} \) of modulus one. The LE vanishes and hence, \textit{all solutions are linearly stable}. Particularly, sensitive dependence with respect to the initial conditions is excluded so that the combined AL-DNLS system possesses only stable regular orbits, whenever the sufficient condition \( E\mu \geq \gamma \) holds. In the parameter range given by the inequality (57), the AL-DNLS chain is transparent (see Section 2.6 below). We note that in the range outside that of the sufficient condition for regularity (\( E\mu \geq \gamma \)), and for the special case of constant amplitude \( \phi_n = \phi_0 \), i.e. for a period-1 cycle, the condition \( |\text{Tr}[M_q]| < 2 \) can be satisfied, if \( |\text{Tr}[J(J(\mathcal{M}_0))]| < 2 \). Especially, for large amplitudes the trace of all local Jacobians \( \tilde{E}_n(\phi_n) = \tilde{E}_0(|\phi_0|) \) becomes a constant

\[
\lim_{|\phi_0| \to \infty} |\tilde{E}_0| = \frac{\gamma}{\mu},
\]

which implies that, if \( \gamma > 0 \) and \( \mu > 0 \) satisfy the inequality

\[
2\mu > \gamma,
\]

the global trace is \( |\text{Tr}[J(J(\mathcal{M}))]| = |2\cos(N\theta)| < 2 \), where \( \theta = \cos^{-1}[\gamma/(2\mu)] \) and the \textit{large amplitude motion is stable} regardless of \( E \).

2.4. Reduction of the dynamics to a two-dimensional map

We now study the dynamics of Eq. (45) utilizing a planar nonlinear dynamical map approach. The discrete nonlinear Schrödinger equation (45) gives a recurrence relation \( \phi_{n+1} = \phi_{n+1}(\phi_n, \phi_{n-1}) \) acting as a four-dimensional mapping \( \mathbb{C}^2 \to \mathbb{C}^2 \). By exploiting the conservation of probability current, the dynamics can be reduced to a two-dimensional mapping on the plane \( \mathbb{R}^2 \to \mathbb{R}^2 \) [81,82]. Following Wan and Soukoulis [82], we use polar coordinates for \( \phi_n \), i.e. \( \phi_n = r_n \exp(i\theta_n) \) and rewrite Eq. (46) equivalently as

\[
r_{n+1} \cos(A\theta_{n+1}) + r_{n-1} \cos(A\theta_n) = \frac{E + \gamma r_n^2}{1 + \mu r_n^2},
\]

\[
r_{n+1} \sin(A\theta_{n+1}) - r_{n-1} \sin(A\theta_n) = 0,
\]
where $\Delta \theta_n = \theta_n - \theta_{n-1}$. Eq. (80) is equivalent to conservation of the probability current

$$J = r_n r_{n-1} \sin(\Delta \theta_n).$$

We further introduce real-valued $SU(2)$-variables defined by bilinear combinations of the wave amplitudes on each “dimeric” segment of the lattice chain:

$$x_n = \phi_n^* \phi_{n-1} + \phi_n \phi_{n-1}^* = 2 r_n r_{n-1} \cos(\Delta \theta_n),$$

$$y_n = i [\phi_n^* \phi_{n-1} - \phi_n \phi_{n-1}^*] = 2 J,$$

$$z_n = |\phi_n|^2 - |\phi_{n-1}|^2 = r_n^2 - r_{n-1}^2.$$

The relations with the polar coordinates $(r_n, \theta_n)$ are also given. Note that the variable $y_n$ is a conserved quantity since it is proportional to the probability current, i.e. $y_n = 2 J$. The variable $z_n$ is determined by the difference of the amplitudes of adjacent lattice sites whereas information about the phase difference is contained in the variable $x_n$. We remark, that our map variables differs from those used by Wan and Soukoulis [82] in their study of the stationary DNLS system.

The system of equations (79) and (80), can be rewritten as a two-dimensional real map $M$ that describes the complete dynamics:

$$M: \begin{cases} x_{n+1} = \frac{E + \frac{1}{2} j (w_n + z_n)}{1 + \frac{1}{2} \mu (w_n + z_n)} (w_n + z_n) - x_n, \\ z_{n+1} = \frac{1}{2} \frac{x_{n+1}^2 - x_n^2}{w_n + z_n} - z_n, \end{cases}$$

with $w_n = \sqrt{x_n^2 + z_n^2 + 4J^2}$.

The map $M$ is reversible, proven by the identities $MM_1M_1 = Id$ and $M_1M_1 = Id$, where the map $M_1$ is

$$M_1: \begin{cases} \hat{x} = x, \\ \hat{z} = -z. \end{cases}$$

We can cast the map $M$ into the product of two involutions $M = AB$ with $A = M_1M_1^{-1}$ and $B = M_1M_2$, and $A^2 = Id$, $B^2 = Id$, and $M_2$ is

$$M_2: \begin{cases} \hat{x} = x, \\ \hat{z} = z. \end{cases}$$

The inverse map is then given by $M^{-1} = BA$. This reversibility property of the map $M$ can be exploited in studying the transmission properties of the discrete nonlinear chain (see Section 2.6).

To analyze the dynamical properties of the nonlinear map $M$ it is convenient to introduce the scaling transformations $2Jx_n \to \tilde{x}_n$, $2Jz_n \to \tilde{z}_n$, $J\gamma \to \tilde{\gamma}$ and $J\mu \to \tilde{\mu}$. Finally, for the sake of simplicity of notation, we drop the overbars and obtain the scaled map

$$x_{n+1} = \frac{E + \gamma (w_n + z_n)}{1 + \mu (w_n + z_n)} (w_n + z_n) - x_n,$$

$$z_{n+1} = \frac{1}{2} \frac{x_{n+1}^2 - x_n^2}{w_n + z_n} - z_n,$$

with $w_n = \sqrt{x_n^2 + z_n^2 + 1}$.
The map $M$ depends on three parameters, namely $(E, \gamma, \mu)$. Whereas for $E\mu \geq \gamma$, $M$ represents a map, for which all solutions are bounded, it can contain bounded and diverging orbits both in the pure DNLS case ($\gamma \neq 0$ and $\mu = 0$) as well as in the combined AL-DNLS case, if $\gamma > 2\mu$ according to the findings in Section 2.3. Only the bounded orbits correspond to transmitting waves, whereas the unbounded orbits correspond to waves with amplitude escaping to infinity and hence do not contribute to wave transmission. On inspection we find the first integral for the AL system to be

$$E^2(x_{n+1}^2 - x_n^2)^2 = [(x_{n+1} + x_n)^2 - K][\mu(x_{n+1}^2 - x_n^2) + 2(z_{n+1} + z_n)]^2,$$  \hspace{1cm} (90)

where $K$ is a constant determined by the initial conditions.

The structure on the phase plane is organized by a hierarchy of periodic orbits surrounded by quasiperiodic orbits. The sets of the corresponding fixed points form the invariant sets of the two involutions (fundamental symmetry lines) and are given by

$$S_0: \quad z = 0,$$  \hspace{1cm} (91)

$$S_1: \quad x = \frac{1}{2} \frac{E + \gamma(w + z)}{1 + \mu(w + z)} (w + z),$$  \hspace{1cm} (92)

respectively. The symmetric periodic orbits are arranged along higher order symmetry lines and the intersection of any two symmetry lines $S_0^n = M^nS_0$, $S_1^n = M^nS_1$ with $n = 0, 1, \ldots$, fall on a periodic orbit of $M$. The symmetry line $z = 0$ is the dominant symmetry line and contains at least one point of every positive residue Poincaré–Birkhoff orbit. The organization of the periodic orbits by the symmetry lines can be exploited for a one-dimensional search to locate any desired periodic orbit on the $x$--$z$ plane [28,30]. For a classification of the periodic orbits Greene’s method can be used according to which the stability of an orbit of period $q$ is determined by its residue $\rho = \frac{1}{2} (2 - \text{Tr} [\prod_{n=1}^q DM^{(n)}])$, where $DM$ is the linearization of $M$. The periodic orbit is stable when $0 < \rho < 1$ (elliptic) and unstable when $\rho > 1$ (hyperbolic with reflection) or $\rho < 0$ (hyperbolic) [28,43].

As can be seen from the determinant of the Jacobian

$$\text{det}(DM^{(n)}) = 1 + \frac{1}{2} \frac{x_{n+1}^2 - x_n^2}{w_n(w_n + z_n)},$$  \hspace{1cm} (93)

the map $M$ is area-preserving for periodic orbits, after mapping through the complete period, i.e. $\prod_{n=1}^q \text{det}(DM^{(n)}) = 1$. $M$ is thus topologically equivalent to an area-preserving map ensuring the existence of KAM-tori near the symmetric elliptic fixed points [44].

2.5. Period-doubling bifurcation sequence

We focus on the period-1 orbits (fixed-points of $M$) which have in the case of elliptic-type stability the largest basins of stability among all elliptic orbits. Thus the stable elliptic solutions encircling the fixed point form the main island on the map plane which plays therefore a major role in determining the stability properties of the wave amplitude dynamics.
The period-1 orbit is determined by

\[ \bar{x} = \frac{1}{2} \frac{E + \gamma \tilde{w}}{1 + \mu \tilde{w}}, \quad (94) \]

\[ \bar{z} = 0, \quad (95) \]

where \( \tilde{w} = \sqrt{1 + \bar{x}^2} \). Eq. (94) possesses one real root for \( \gamma = 0 \), resulting in a stable elliptic fixed point and has either no root or two real roots for \( \gamma > 0 \). The two real roots correspond to one hyperbolic and one elliptic fixed point, respectively. The residue is given by

\[ \rho = 1 - \frac{1}{2} \frac{(E + \gamma \tilde{w})(E + 2\gamma \tilde{w} + \gamma \mu \tilde{w})}{(1 + \mu \tilde{w})^3}. \quad (96) \]

When, \( \gamma = E\mu \), we recover the degenerate linear case, for which \( \bar{x} = \text{sign}(E)\sqrt{E^2/(4 - E^2)} \) and \( \rho = 1 - E^2/4 \), like in the genuine linear case \( \gamma = \mu = 0 \).

Concerning the stability of the period-1 orbit, Eq. (96) tells us that the residue remains positive and never passes through zero, if the parameters obey the inequalities \( \gamma < E\mu \) and \( |E| < 2 \). As a result, the period-1 orbit cannot lose stability caused by a tangent bifurcation. According to the results obtained in Section 2.3, all orbits of the map are regular in this parameter range.

Eq. (96) allows a further conclusion to be drawn: For \( E > 0 \) the value of the residue for the period-1 orbit is always less than one, because the second term on the right-hand side then remains positive upon parameter changes and the position of the fixed point is merely shifted and never experiences loss of stability due to a period-doubling bifurcation. In this parameter range the route to global chaos is via resonance overlap. Only for \( E < 0 \) can the residue pass the value of one connected with the onset of a period-doubling bifurcation, where the stable fixed point is converted into an unstable hyperbolic point with reflection accompanied by the creation of two additional elliptic points. This period-doubling bifurcation for the period-1 orbit sets in when \( |E|/\gamma > 1 \) \( (E < 0) \) and the newborn period-2 orbits are located at

\[ x = \pm \sqrt{(E/\gamma)^2 - 1}, \quad (97) \]

\[ z = 0. \quad (98) \]

Note that the location of the period-2 orbits depends only on the \((E, \gamma)\) values and is independent of \( \mu \), the AL-nonlinearity strength, whereas their stability, determined by the corresponding residue

\[ \rho = \frac{1}{2} \frac{\gamma^2 (E^2 - \gamma^2)}{(\gamma + \mu |E|)^2}, \quad (99) \]

depends on the values of all three parameters. Due to the presence of the denominator in Eq. (99) we recognize that, for fixed parameters \((E, \gamma)\), enhancing the \( \mu \) value reduces the residue. Hence, the period-2 orbits become more resistant with respect to period-doubling bifurcation. Moreover, for \( \mu > \mu_c \) the value for the residue of the two stable elliptic points is bounded from above by one, so that a further destabilizing bifurcation can be excluded. This critical AL-nonlinearity strength \( \mu_c (\rho < 1) \) can be obtained as

\[ \mu_c > \frac{1}{2} \frac{\gamma^2 (1 - (\gamma/E)^2)}{|E|} - \frac{\gamma}{|E|}. \quad (100) \]
To study the period-doubling sequence as the mechanism by which the transition from regular to chaotic motion occurs, we take advantage of the renormalization technique developed for two-dimensional invertible maps [28–30, 33, 94]. We expand the map \( M \) up to terms quadratic in the deviation from the bifurcation point

\[
\begin{pmatrix}
\delta u_{n+1} \\
\delta v_{n+1}
\end{pmatrix} = \mathcal{A} \begin{pmatrix}
\delta u_n \\
\delta v_n
\end{pmatrix} + \mathcal{B} \begin{pmatrix}
\delta u_n^2 \\
\delta v_n^2
\end{pmatrix},
\tag{101}
\]

The \( 2 \times 2 \) matrix \( \mathcal{A} \) has the following entries:

\[
\mathcal{A}_{11} = -1, \quad \mathcal{A}_{12} = \frac{E + 2\gamma + \mu^2}{[1 + \mu]^2},
\]

\[
\mathcal{A}_{21} = -\frac{E + \gamma}{1 + \mu}, \quad \mathcal{A}_{22} = \frac{1}{2} \left[ \frac{E + \gamma}{1 + \mu} \right] \left[ \frac{E + 3\gamma + \gamma \mu - E \mu}{[1 + \mu]^3} \right] - 1,
\tag{102}
\]

and the elements of the \( 2 \times 3 \) matrix \( \mathcal{B} \) are given by

\[
\mathcal{B}_{11} = \mathcal{A}_{12}, \quad \mathcal{B}_{12} = 0,
\]

\[
\mathcal{B}_{21} = \mathcal{A}_{22} + 1, \quad \mathcal{B}_{22} = \mathcal{A}_{12},
\]

\[
\mathcal{B}_{13} = \frac{E + 4\gamma + 3\gamma \mu - E \mu + \gamma^2 \mu^2}{[1 + \mu]^3},
\]

\[
\mathcal{B}_{23} = \frac{1}{2} \frac{E^2 + 8\gamma - 4E \gamma \mu + 9\gamma^2 + \gamma^2 \mu^2 - 4E^2 \mu + \mu^2 E^2}{[1 + \mu]^4}.
\tag{103}
\]

Finally, we bring the De Vogelaere-type map (101) into the standard form of a closed second-order difference equation (see Ref. [33] for the details how to achieve this form):

\[
Q_{n+1} + Q_{n-1} = CQ_n + 2Q_n^2,
\tag{104}
\]

where the parameter \( C \) is determined via the sum of the eigenvalues of the matrix \( \mathcal{A} \):

\[
C = \frac{1}{4} \frac{[E + \gamma] [E + 3\gamma + \gamma \mu - E \mu]}{[1 + \mu]^3} - 1.
\tag{105}
\]

The fixed point of equation (104) at \( \bar{Q} = 0 \) is stable for \( |E|/\gamma < 1 \) and gets unstable for \( 3 > |E|/\gamma > 1 \) leading to a period-doubling bifurcation. Both points of the newborn period-2 orbit are located on the \( S_0 \)-symmetry line, along which they get shifted upon increasing \( |E| \). Eventually, at a sufficiently high \( |E| \) value the period-2 orbit also loses stability caused by a next period-doubling bifurcation, which in turn gives rise to the birth of the corresponding period-4 orbit having one point on the \( S_1 \)-symmetry line and two points on the \( S_0 \)-symmetry line. For further increased \( |E| \) the period-4 orbit also goes unstable in the next step of the period-doubling cascade.

This cascade of period-doubling bifurcations terminates at a universal critical parameter \( C_\infty \), called the accumulation point, where local chaos appears. Employing a quadratic renormalization scheme for Eq. (104), this accumulation point has been determined to be \( C_\infty \approx -1.2656 \).
[28–30,33,94]. Solving Eq. (105) for $E_\infty = E(\gamma, \mu, C_\infty)$ we obtain

$$E_\infty = -\frac{1}{1-\mu}[2\gamma + (1+\mu)\sqrt{\gamma^2 - |C_\infty|(1-\mu^2)^2}] .$$

(106)

Apparently, for a given DNLS-nonlinearity strength $\gamma$, we conclude that enhancing the AL-nonlinearity strength $\mu$ results in an increase of the accumulation value $|E_\infty|$ (provided $\mu < 1$), i.e. the $\mu$ term has the stabilizing tendency to prevent period-doubling sequences.

In Fig. 3a we show a number of orbits of the map $M$ for $E = 0.5$, $\gamma = 0.2$ and $\mu = 0.1$ together with the symmetry lines $S_0$ and $S_1$. This map exhibits a rich structure involving regular

---

**Fig. 3.** Orbits of the map $M$ given in Eqs. (88) and (89) for the parameters: (a) AL-DNLS case: $E = 0.5$, $\gamma = 0.2$ and $\mu = 0.1$. (b) AL case: $E = -1.0$, $\gamma = 0$ and $\mu = 1.0$. Superimposed in (a) are also the fundamental symmetry lines $S_0$ and $S_1$. 

quasiperiodic (KAM) curves which densely fill the large basin of attraction of the stable period-1 orbit. The elliptic fixed points of the Poincaré–Birkhoff chains of various higher-order periodic orbits are also surrounded by regular KAM curves, while thin chaotic layers develop in the vicinity of the separatrices of the corresponding hyperbolic fixed points. Moreover, outside the structured core containing trapped trajectories inside the resonances, a broad chaotic sea has been developed where the corresponding unstable orbits may escape to infinity. For comparison we illustrate in Fig. 3b the integrable behavior for the AL-map where the corresponding orbits can be generated from Eq. (90).

In order to study the global stability properties of the map $M$, we plotted in Fig. 4 the stability diagram in the $x_0$–$E$ plane. For a set of initial conditions located on the dominant symmetry line, i.e. $z = z_0 = 0$ and various $x = x_0$, we iterated the map Eqs. (88) and (89). The dark region in Fig. 4 corresponds to stable solutions where the resulting orbit remains in a bounded region on the $x$–$z$ plane of the map, whereas the white region on the $x_0$–$E$ plane represents unbounded orbits. The curve separating the two regimes exhibits a rich structure. Practically, all lines of constant $E$ pass several branches of either transmitting or nontransmitting solutions indicating multistable behavior. Multistability in the wave transmission along the nonlinear lattice chain will be considered in more detail in the next section.

We further note that with increasing AL-nonlinearity parameter $\mu$ the area of transmitting solutions on the $E$–$x_0$ plane enhances. Beyond a certain nonlinearity strength $\mu \geq \gamma/E$, the nonlinear lattice chain eventually becomes transparent for all amplitudes.

In Fig. 4a we also superimposed the line for the location of the fixed point (period-1 orbit) of the map $M$. Following that line the occurring transition from a bounded to an unbounded regime for initial conditions around the period-1 orbit is a consequence of stability loss when passing from elliptic-type stability to hyperbolic-type instability upon changing $E$. They may experience a bifurcation from an unstable hyperbolic fixed point to a stable elliptic fixed point by increasing $E$ where the corresponding $x_0$ values then come to lie in the basin of attraction of the elliptic point. At a critical $E$ value the initial conditions $x_0$ leave the basin of attraction of the elliptic point and fall into the range of the unstable reflection hyperbolic point. Between the lower and the upper stability boundaries the elliptic point loses its stability temporarily caused by a quadrupling-bifurcation where the corresponding residue is $\rho = 0.75$ leading to a local shrinkage of the area for bounded solutions which appears in Fig. 4a for $E \approx -1.075$ and $x_0 \approx 0.24$.

### 2.6. Transmission properties

In this section we study as a physical application the wave transmission properties of the nonlinear lattice chain. Our aim is to gain more insight into the effects of the combined AL-nonlinearity term and the DNLS-nonlinearity term with regard to wave transparency of a finite nonlinear segment embedded in a linear chain.

Since the work of Winful et al. it is known that periodic modulation of a nonlinear medium leads to bistable behavior and the transmitted intensity of an incident plane wave on an finite one dimensional nonlinear medium is no longer a unique function of the input intensity [109]. Delyon et al. [81] have shown that the transmission of a wave through a (finite) sample of periodic nonlinear medium such as the DNLS exhibits nonanalytical properties. The transmission properties are further characterized by multistability induced by the spatial periodic modulation of the
medium due to the lattice discreteness in addition to the nonlinearity. They found that the transmitted energy exhibits plateaus as a function of the incident intensity and the frequency versus intensity propagation diagram is fractal. Kahn and co-workers studied the nonlinear optical response of a superlattice constructed of alternating layers of dielectric, and an (insulating) antiferromagnetic film and observed also multistability and transmittivity gaps [96] (see also below).
2.7. Amplitude stability

We study the following transmission problem: Plane waves with momentum $k$ are sent from the left towards the nonlinear chain, where they will be scattered into a reflected and transmitted part:

$$\phi_n = \begin{cases} R_0 \exp(ikn) + R \exp(-ikn) & \text{for } 1 \leq n \leq N, \\ T \exp(ikn) & \text{for } n \geq N. \end{cases}$$

We denote by $R_0$, $R$ the amplitudes of the incoming and reflected waves and by $T$ the transmitted amplitude at the right end of the nonlinear chain. The wave number $k$ is in the interval $[-\pi, \pi]$ yielding $|E| \leq 2$.

Since the superposition principle is no longer valid in the nonlinear case, the transmitted amplitude $T$ is not uniquely defined by the incident amplitude $R_0$. To circumvent this difficulty we solve the inverse transmission problem, i.e. compute the input amplitude $R_0$ for fixed output amplitude $T$ (see also [81]). The procedure relies on the inverse map given by $M^{-1} = M_1MM_1$ which we interpret as a “backward map” in the following manner: For a given output plane wave with transmitted intensity $T$ at the right end of the nonlinear chain we have $(\phi_{N+1}, \phi_N) = [T \exp(ik(N + 1)), T \exp(ikN)]$. From the pair $(\phi_{N+1}, \phi_N)$ we obtain $(r_{N+1}, r_N)$ and $(\theta_{N+1}, \theta_N)$ as well as $(x_{N+1} = 2T^2 \cos(k), z_{N+1} = 0)$. The latter are used as initial conditions for the map $M^{-1}$ in the study of the fixed output transmission problem. For a given wavenumber $k$ the current $J$ is fixed through the expression $J = |T|^2 \sin(k)$. We see, therefore, that the pair $(k, |T|)$ initializes the map $M^{-1}$ completely. Iterating the map $M^{-1}$ from $n = N$ to $n = 0$ successively determines the amplitudes $(r_{N-1}, \ldots, r_0)$ and phases $(\theta_{N-1}, \ldots, \theta_0)$ and eventually results in the value of $\phi_0$ on the left end of the nonlinear chain.

Fig. 5 displays the transmission behavior in the $k - |T|$ parameter plane (momentum versus intensity amplitude of an outgoing wave), showing regions of transmitting (white) and nontransmitting (hatched) behavior. This representation is similar to that used by Delyon et al. and Wan and Soukoulis in the study of the corresponding stationary DNLS-model [81,82].

For a given output wave with intensity $|T|$ and momentum $k$ the inverse map $M^{-1}$ has been iterated by taking a grid of 500 values of $k$ and 250 values $|T|$. Correspondingly, to initialize the map $M^{-1}$ we populate the $z$-axis with initial conditions $x_0 = 2|T| \cos(k)$, $z_0 = 0$ and iterate on each individual point. When the resulting incoming wave intensities $|R_0|$ are of the same order of magnitude as the transmitted intensity, the nonlinear chain is said to be transmitting (white area in Fig. 5). In Fig. 5 we show the AL-DNLS case $\mu = 0.25$, with $\gamma = 1$.

For wave numbers $|k| \in [\pi/2, \pi]$ the regions of bounded and unbounded solutions are separated by a sharp smooth curve which can be obtained approximately from the analysis for the initial wave amplitude stability performed in Section 2.3. Using Eq. (73) the boundary follows from

$$|\phi_T| = \frac{1}{\mu} \left\{ \sqrt{1 + \frac{2\mu(1 - \cos(k))}{\gamma - 2\mu}} - 1 \right\},$$

where $\phi_T$ is the critical value for the wave amplitude above which stable transmission is necessarily impossible.
As AL-nonlinearity increases its stabilizing effect manifest itself in an area enhancement of the region for transmitting solutions. This effect becomes more pronounced for higher AL-nonlinearity strength (not shown here), eventually exhibiting perfect transmittance, when $E\mu \geq \gamma$

For $|k| < \pi/2$ the region for nontransmitting solutions ranges down into the region of linearly transmitting solutions, thus decreasing transparency. The boundary discerning between bounded and unbounded solutions shows a complex structure created by numerous narrow hatched tongues. The white regions between each of these tongues can be assigned to a corresponding stability basin of an elliptic periodic orbit and the fractal structure of the boundary curves originates from the hierarchical, self-similar structure of islands around islands formed by higher-class periodic orbits [81,82].

In the transmission diagrams represented in Fig. 5, several branches are created for $k \in [-\pi/2, \pi/2]$ at critical intensities $|T|$, indicating bistable or multistable behavior. Such multistability is illustrated in Fig. 6, where the transmitted wave intensity is plotted versus the intensity of the incoming wave for $k = 0.927$. The curve in Fig. 6a illustrating the pure DNLS case ($\gamma = 1.0$, $\mu = 0$) shows oscillations resulting in numerous different output energies for a given input energy. Above an output intensity of 0.68, a transmission gap ranging up to 1.08 occurs. Fig. 6b demonstrates that the presence of a stabilizing AL nonlinearity of $\mu = 0.5$ closes the gap, i.e. transmittivity of the nonlinear lattice is restored.

We presented an investigation of the nonlinear stationary problem of a discrete nonlinear equation that interpolates between the Ablowitz–Ladik and discrete nonlinear Schrödinger equation utilizing map approaches. The different regimes of the dynamical system were seen to depend on the two nonlinearity parameters $\mu$ and $\gamma$ as well as the wave energy $E$. Using the properties of the
Fig. 6. Transmitted intensity as a function of the incident intensity exhibiting multistability of the nonlinear transmission dynamics for a nonlinear chain consisting of 200 sites. The parameters are $E = -1.2$, $c = 1.0$, and (a) $k = 0$. A transmission gap occurs. (b) The gap has been closed for $k = 0.5$.

In the tangent space map we found that, when $E\mu \geq \gamma$ is satisfied, all orbits are characterized by a (largest) Lyapunov exponent that is equal to zero, thus leading to stable solutions. Consequently, this inequality marks the regime where transmission through the nonlinear lattice is ensured. Furthermore, for waves with energies outside this regime we found that stable map solutions are also guaranteed when $2\mu > \gamma$. The existence of these regular regimes shows that the presence of the AL term in Eq. (45) has the significant function of creating an “integrability regime” for the nonintegrable DNLS. We studied also the transmission properties of Eq. (45) in two ways and showed that in addition to the regular transparent regimes, there are also cases where multistability is possible. The effect of the AL term is to close the transmission gaps and thus enhances the transparency of the nonlinear lattice [83].
3. Soliton-like solutions of the generalized discrete nonlinear Schrödinger equation

3.1. Introduction

In this chapter we study the localized stationary solutions of the GDNLS equation in the real domain in greater detail. We show that the results of the stationary analysis can be used to excite localized stationary states of designed patterns on the lattice. Stationary localized solutions of a pure DNLS system were studied in [82,107,108] in the context of wave propagation in periodically modulated media. In nonlinear optics Kerr type nonlinearities give rise to DNLS equations and the localized solutions are supported by states in the first gap, therefore called gap solitons [34,95,96,110,112–114]. The corresponding stationary system can be treated by a nonlinear map approach. In searching for localized solutions one has to be aware that the stationary nonintegrable DNLS system exhibits irregular chaotic behavior which led the authors of [82,107,108] to the conclusion that perfect localization in a nonintegrable lattice system is impossible. Nevertheless, we demonstrate that stable localized lattice states conspire with the nonintegrability of the map orbits through homoclinic and heteroclinic connections.

The chapter is organized as follows: In Section 3.2 we introduce the real-valued stationary AL-DNLS problem and link it with a two-dimensional area-preserving map. We discuss the stability properties of the fixed points of the map. In Section 3.3 we discuss the anti-integrable limit of the GDNLS and prove the existence of localized solutions. In Section 3.4 the Melnikov method is used to prove the existence of homoclinic orbits thus showing nonintegrability of the map. With the help of the Birkhoff normal forms we determine homoclinic orbits analytically in Section 3.5 and compute the soliton pinning energy. In order to obtain the heteroclinic orbits we exploit a variational approach relating the heteroclinic points to the critical points of a certain action function. In Section 3.6 we excite bright (dark) solitons in the dynamical DNLS using the homoclinic (heteroclinic) map orbits as initial data. Finally, in Section 3.8 we give a short summary. (Also, see Refs. [99–103,105,106,116].)

3.2. The real-valued stationary problem of the GDNLS

We investigate the solution properties of the GDNLS where we focus on time-periodic but spatially localized solutions [115]. As is shown below such a study of localized GDNLS states implies real-valued stationary amplitudes. Substituting the ansatz

$$\psi_n(t) = \phi_n \exp(-i\omega t),$$

with amplitudes $\phi_n$ and the phase (oscillation frequency) $\omega$ into Eq. (44), we obtain the following coupled system for the amplitudes $\phi_n$:

$$\omega \phi_n + \gamma |\phi_n|^2 \phi_n + (V + \mu |\phi_n|^2)(\phi_{n+1} + \phi_{n-1}) = 0.$$  (109)

To distinguish the present study (in the real domain) from those performed in the preceding chapter (in the complex domain) we use for the stationary phase the notation $\omega$. We further remark that for computational convenience the current sign convention for the dispersion term is chosen to be opposite to those of the stationary Eq. (45).
We are particularly interested in solutions exponentially localized at a single site and distinguish two situations: (1) $|\phi_n| > |\phi_{n+1}|$ for $n > 0$ and $|\phi_n| < |\phi_{n+1}|$ for $n < 0$ with $\lim_{|n| \to \infty} |\phi_n| = 0$ corresponding to the bright soliton-like solution, and (2) $|\phi_n| < |\phi_{n+1}|$ for $n > 0$ and $|\phi_{n+1}| < |\phi_n|$ for $n < 0$ with $\lim_{|n| \to \infty} |\phi_n| = a > 0$ resulting in the dark soliton-like solution. Without loss of generality we assume that both types of the soliton-like solutions have their main deviations from the background around the central element of the lattice. Furthermore we request for the bright (dark) soliton solution exponential decrease (increase) of the amplitudes apart from the central site for $|n| \to \infty$.

It can be readily seen that the current $J$ defined by

$$J = i \left[ \phi_n^* \phi_{n-1} - \phi_n \phi_{n-1}^* \right]$$

is conserved for the system of the stationary equations. Since we consider an open lattice chain (without periodic boundary conditions) we can show that localized solutions implies real amplitudes $\phi_n \in \mathbb{R}$. To this end we consider the value for the current at one of the ends of the chain assumed to be of finite length $N$ for the moment. Representing $\phi_{N-1}$ by the r.h.s. of the corresponding stationary equation

$$V \phi_{N-1} = -\frac{\omega + \gamma |\phi_N|^2}{V + \mu |\phi_N|^2} \phi_N,$$

we immediately obtain that $J \equiv 0$. Due to the conservation of $J$ this result must hold for all lattice indices $n \in [-N, N]$ which however can only be fulfilled for either the special case of constant amplitudes $\phi_n = \text{constant}$ or, in general, only for real-valued $\phi_n \in \mathbb{R}$. The last result is independent of the value of $N$. Hence, for the remainder of this chapter we consider real-valued amplitudes $\phi_n$.

It is convenient to cast the real-valued second-order difference equation (109) into a two-dimensional map $\mathbb{R}^2 \to \mathbb{R}^2$ by defining $x_n = \phi_n$ and $y_n = \phi_{n-1}$ where the lattice index plays the role of discrete “time”. We arrive at the map:

$$\mathcal{M}: \begin{cases} x_{n+1} = -\frac{\omega + \gamma x_n^2}{1 + \mu x_n^2} x_n - y_n, \\ y_{n+1} = x_n. \end{cases}$$

We used the notation $\tilde{\omega} = \omega/V$ and $\tilde{\gamma} = \gamma/V$ and the tildes are conveniently dropped afterwards. Reversibility of the map $\mathcal{M}$ is established by the factorization $\mathcal{M} = \mathcal{M}_0 \mathcal{M}_1$ with

$$\mathcal{M}_0: \begin{cases} \tilde{x} = y, \\ \tilde{y} = x, \end{cases}$$

$$\mathcal{M}_1: \begin{cases} \tilde{x} = x, \\ \tilde{y} = -\frac{\omega + \gamma x^2}{1 + \mu x^2} - y, \end{cases}$$

where $\mathcal{M}_{0,1}$ are involutions and their corresponding symmetry lines are given by $S_0: x = y$ and $S_1: y = -(1/2)(\omega x + \gamma x^3)/(1 + \mu x^2)$. Furthermore, the map $\mathcal{M}$ is an analytic area-preserving map.

In order to investigate stationary localized solutions in the form of the bright (dark) soliton, respectively, it suffices to study the fixed points (period-1 orbits) of the map $\mathcal{M}$. The fixed points, for
which \( \hat{x} = \hat{y} \), of this map are located at

\[
\hat{x}_0 = 0, \quad \hat{x}_\pm = \pm \sqrt{-\omega + 2/\gamma + 2\mu},
\]

(115)

where \( \hat{x}_\pm \) exists only if \( \text{sign}(\omega + 2) = -\text{sign}(\gamma + 2\mu) \). The stability of the fixed points is governed by their value for the corresponding residues \([28,43]\) \( \rho = 1/4 [2 - \text{Tr}(D.\mathcal{M}(\hat{x}))] \). The tangent map \( D.\mathcal{M} \) is determined by

\[
D.\mathcal{M}(x) = \begin{pmatrix} \omega_n & -1 \\ 1 & 0 \end{pmatrix},
\]

(116)

with

\[
\omega_n = -\frac{\omega + (3\gamma - \mu\omega)x_n^2 + \gamma\mu x_n^4}{(1 + \mu x_n^2)^2}.
\]

(117)

The residue corresponding to the fixed point at the origin is

\[
\rho = \frac{1}{4}(\omega + 2).
\]

(118)

For \( \omega \) values within the range of the linear band, i.e. \(|\omega| < 2, 0 < \rho < 1 \) holds and the origin is a stable elliptic fixed point encircled by stable elliptic type map orbits. For \(|\omega| > 2 \) (outside the range of the linear band) we distinguish the following two cases:

(i) \( \omega < -2, \gamma + 2\mu > 0 \).

In this case the residue passes through zero, i.e. \( \rho < 0 \), and hence the origin loses stability and is turned into an unstable hyperbolic point caused by a tangent bifurcation. This hyperbolic point is connected to itself by a homoclinic orbit created by the (invariant) unstable and stable manifold. As will be shown below the homoclinic orbit is manifested on the lattice chain as a \textit{soliton-like solution} which is equivalent to the so called gap soliton of nonlinear optics lying in the stop band below the linear passing band \([34,112,71]\).

The pair of points \( \hat{x}_\pm \) on the symmetry line \( S_0 \) form stable elliptic fixed points.

(ii) \( \omega > 2, \gamma + 2\mu < 0 \).

The value for the residue at the origin passes through the value of one, that is \( \rho > 1 \), connected with the onset of a period-doubling bifurcation, where the fixed point is converted into an unstable hyperbolic point with reflection. The newly created period-2 orbits are located on the line \( x = -y \).

The homoclinic map orbit supports on the lattice chain a soliton-like solution which exists in the gap above the linear passing band and has alternating signs for adjacent amplitudes, i.e. \( \text{sign}(\phi_{n+1}) = -\text{sign}(\phi_n) \) as a characteristic feature (see below). This stationary localized structure has been called a \textit{staggered soliton} by Cai et al. in their study of the combined AL-DNLS equation \([18]\). Correspondingly the soliton solution of case (ii) is called unstaggered soliton. Note that upon sign change \( \gamma \rightarrow -\gamma \) and \( \omega \rightarrow -\omega \) the map has the symmetry property of \( \text{sign}(\phi_{n+1}) = -\text{sign}(\phi_n) \) so that the unstaggered and staggered soliton replace each other. A third case of unstable fixed points can also be attributed to the occurrence of a stationary localized structure on the nonlinear lattice, namely:

(iii) \(|\omega| < 2 \) and \( \gamma + 2\mu < 0 \).

Since the frequency is in the linear band the origin is still a stable elliptic fixed point whereas the pair of fixed points \( \hat{x}_\pm \) on the symmetry line \( S_0 \) represents two unstable hyperbolic fixed points.
which are connected to each other via a (pair of) heteroclinic orbits. This heteroclinic map orbit represents a kink-like solution, also called a dark soliton. There exist staggered and unstaggered versions of this soliton, too.

3.3. The anti-integrable limit and localized solutions

In this section we apply the concept of the anti-integrable limit introduced by Aubry and Abramovici [117,118]. We are particularly interested in the impact of the integrable AL term of Eq. (44) on the formation of breathers, i.e. the occurrence of time-periodic, spatially localized solutions. Recently, MacKay and Aubry have proven the existence of localized solutions in form of breathers for weakly coupled arrays of oscillators [119]. These authors suggested also the application of the anti-integrable (or better called no-coupling) limit to prove the existence of breather solutions for the DNLS system (cf. Section 9 of Ref. [119]). Using the anti-integrable limit Bressloff proved the existence of localized ground states for the standard di\texttimes;usive Haken model describing a neural network [120]. Due to the formal equivalence of the Haken model to a DNLS-Hamiltonian one can also infer from Bressloff’s result on the existence of (stationary) breathers for the DNLS. However, the present study involves besides the nonintegrable DNLS term also additionally the integrable AL contribution. It is worth mentioning that the AL system by itself has no anti-integrable limit.

The spatial behavior of the breathers $\psi_n(t) = \exp(-i\omega t) \phi_n$ of the GDNLS is described by a stationary equation with real amplitudes $\phi_n \in \mathbb{R}$ [119] (see also discussion above). Since $|\psi_n(t)|^2 = \phi_n^2$ does not change with time these solutions can be viewed as static breathers. The action for the real-valued AL-DNLS system reads

$$F = \sum_n \left\{ -\frac{1}{2\mu} \left( \omega - \frac{\gamma}{\mu} \right) \ln(1 + \mu \phi_n^2) - \frac{\gamma}{2\mu} \phi_n^2 + \frac{V}{2}(\phi_{n+1} - \phi_n)^2 \right\}.$$  \hspace{1cm} (119)

(We shifted the linear band by $2V$.) The map orbits are determined by

$$V(\phi_{n+1} + \phi_{n-1} - 2\phi_n) = -\frac{\omega + \gamma \phi_n^2}{1 + \mu \phi_n^2} \phi_n.$$  \hspace{1cm} (120)

The anti-integrable limit for the AL-DNLS system is obtained for vanishing hopping parameter $V = 0$, where the action is represented as the sum over local on-site potentials $U(\phi_n)$:

$$F_{\text{AI}} = \sum_n \left\{ \frac{1}{2\mu} \left( \omega - \frac{\gamma}{\mu} \right) \ln(1 + \mu \phi_n^2) + \frac{\gamma}{2\mu} \phi_n^2 \right\}$$  \hspace{1cm} (121)

$$\equiv \sum_n U(\phi_n).$$  \hspace{1cm} (122)

The orbits for the stationary problem are determined by

$$\frac{\partial U(\phi_n)}{\partial \phi_n} \equiv U'(\phi_n) = 0,$$  \hspace{1cm} (123)

yielding the rest positions

$$\bar{\phi}_0 = 0, \quad \bar{\phi}_\pm = \pm \sqrt{-\omega/\gamma}, \quad \omega < 0, \; \gamma > 0.$$  \hspace{1cm} (124)
Since orbit points at sites \( n + 1 \) and \( n \) are mutually independent of each other an orbit can be associated with an arbitrary sequence of three symbols assigned to \( (\tilde{\phi}_0, \tilde{\phi}_\pm) \). Hence, the orbits are trivially equivalent to a Bernoulli shift establishing the existence of chaotic orbits [117,118]. We can prove that some chaotic solutions of the anti-integrable limit persist, at least up to a critical value \( V_{\text{crit}} \).

**Theorem.** For

\[
V_{\text{crit}} \leq \frac{|U'(|u_\pm|)|}{4\phi_{\text{max}}}
\]

(125)

there exists a unique solution of Eq. (120) such that for all \( n \) deviations from the rest position \( \tilde{\phi}_0 \) are bounded by

\[
|\phi_n| \leq u_+ ,
\]

(126)

and deviations from \( \tilde{\phi}_\pm \) lie in the range given by

\[
\phi_{\text{min}} \leq |\phi_n| \leq \phi_{\text{max}} ,
\]

(127)

with

\[
u_\pm = \pm \left\{ \frac{1}{2\gamma} \left[ \left( \omega - \frac{3\gamma}{\mu} \right) + \sqrt{\omega^2 + \left( \frac{3\gamma}{\mu} \right)^2 - 10\omega \frac{\gamma}{\mu}} \right] \right\}^{1/2} ,
\]

(128)

\[
\phi_{\text{min}} = \left\{ \frac{1}{2\gamma} \left[ 8V_{\text{crit}} + \omega - \frac{3\gamma}{\mu} + \sqrt{\left( \frac{3\gamma}{\mu} - \omega - 8V_{\text{crit}} \right)^2 + 16\gamma V_{\text{crit}} - 4\gamma \omega} \right] \right\}^{1/2} ,
\]

(129)

and \( \phi_{\text{max}} \) is the maximum positive root of the equation

\[
U(\phi_n) = U(u_+) .
\]

(130)

**Proof.** Eq. (120) can be rewritten as

\[
V(\phi_{n+1} + \phi_{n-1} - 2\phi_n) = U'(\phi_n) .
\]

(131)

From Eq. (127) we obtain that

\[
\sup_n |\phi_{n+1} + \phi_{n-1} - 2\phi_n| \leq 4\phi_{\text{max}} ,
\]

(132)

which yields

\[
4V\phi_{\text{max}} \geq |U'(\phi_n)| .
\]

(133)

When

\[
V_{\text{crit}} < \max_n |U'(\phi_n)| = \frac{|U'(|u_\pm|)|}{4\phi_{\text{max}}} ,
\]

(134)

then Eq. (120) has infinitely many solutions. But, in each interval given by the inequalities (126) and (127), there is one and only one solution and hence, the problem is uniquely defined.
From the graph of \( U'(\phi_n) \) it can be readily seen that \( U''(\phi_n) > 0 \) in the interval given by Eq. (126). Further, when (127) holds then \( U'(\phi_n) < -4V \). The Jacobian operator \( D^2F \) is tridiagonal with diagonal elements \( U'' + 2V \) and off-diagonal elements \(-V\). Since \(|U'' + 2V| > 2V\), the operator \( D^2F \) is invertible and its inverse is bounded. Hence it follows from the implicit function theorem that an orbit has a locally unique continuation for \( V < V_{\text{crit}} \) [117–123].

It can easily be shown that \( \partial V_{\text{crit}}/\partial \mu < 0 \) and \( \partial \phi_{\text{max}}/\partial \mu < 0 \). From this we note that the presence of the integrable AL-term has a destabilizing influence on the continuation process of the solutions of the anti-integrable limit in the sense that, the higher the \( \mu \)-values are the lower become the \( V \)-values to which the continuation can be carried out. Moreover, the possible maximal amplitudes \( \phi_{\text{max}} \) of the continued solutions decrease with increasing \( \mu \). An interesting case arises when in the no-couling limit \( V = 0 \) only one site is excited while all the others remain unexcited (e.g. \( \phi_0 = \tilde{\phi}_+ \) and \( \phi_n \neq 0 \)). This results in a so called one-site breather which is maintained under the action of the coupling \( 0 < V < V_{\text{crit}} \) and its spatially exponential localization can be proven with the help of Theorem 3 of [119].

3.4. The Melnikov function and homoclinic orbits

As is well known in generic nonintegrable maps the stable and unstable manifolds of hyperbolic equilibria cross each other in homoclinic points; or there might appear crossings of the stable and the unstable manifolds of different hyperbolic points, called heteroclinic connections. Such two-dimensional maps are often associated with the Poincaré map of periodically perturbed two-dimensional flows [28]. For these time-continuous flows the Melnikov function proved to be a powerful method to show the existence of orbits homoclinic to a hyperbolic equilibrium. Glasser et al. [124] extended the Melnikov analysis to two-dimensional discrete maps of the plane which are of the form \( u_{n+1} = F(u_n) + \varepsilon G(u_n) \) with \( u = (x, y) \in \mathbb{R}^2 \). Thus the r.h.s. is assumed to consist of a completely integrable part \( F \) and a small nonintegrable perturbation \( \varepsilon G \) with \( \varepsilon \ll 1 \). Furthermore, the unperturbed system of \( \varepsilon = 0 \) possesses an unstable equilibrium characterized by coinciding stable and unstable manifolds forming a perfect unperturbed separatrix on which the solution is known explicitly. Based on geometric arguments a Melnikov function was developed in [124] measuring the distance between the stable and unstable manifolds under the action of the perturbation.

For a perturbational treatment we consider the nonlinear term related with \( \gamma \) as a small (nonintegrable) perturbation of the integrable AL map \( (\gamma = 0, \mu \neq 0) \). Therefore we introduce in Eq. (112) the small parameter \( \varepsilon \):

\[
x_{n+1} = -\frac{\omega + \varepsilon \gamma x_n^2}{1 + \mu x_n^2} - y_n,
\]

\[
y_{n+1} = x_n,
\]

whose integrable part \( (\varepsilon = 0) \) possesses a separatrix given by

\[
\mu x^2 y^2 + x^2 + y^2 + \omega xy = 0.
\]
In the first quadrant the separatrix loop can be parameterized by

\[ x_n(t) = \frac{1}{\sqrt{\mu}} \sinh \beta \text{sech}(t - n\beta), \quad (137) \]

\[ y_n(t) = \frac{1}{\sqrt{\mu}} \sinh \beta \text{sech}(t - (n + 1)\beta), \quad (138) \]

where \( \cosh \beta = -\omega/2 \) and \( t \) is a real parameter regulating the position on the separatrix loop. Note that the AL soliton center of \( x_0(0) = \sqrt{(\omega^2/4 - 1)/\mu} \) and \( y_0(0) = -2x_0(0)/\omega \) is determined on the map plane by the intersection point of the AL separatrix loop with the symmetry line \( S_1 \).

According to [124] the Melnikov function is given by

\[ M(t; \omega, \mu, \gamma) = ||u_0(t)||A'(0), \quad (139) \]

with

\[ A'(0) = \sum_{k = -\infty}^{\infty} G(x_{k-1}, y_{k-1}) \wedge v_k, \quad (140) \]

where the wedge product is \((u_1, u_2) \wedge (v_1, v_2) = u_1v_2 - u_2v_1\). Therefore the unit tangent vector to the separatrix is given as

\[ v_k(t) = u_k(t)/||u_0(t)||, \quad (141) \]

where

\[ u_k(t) = \left( -y_k - \frac{\omega}{2}x_k - \mu x_k^2 y_k, x_k + \frac{\omega}{2}y_k + \mu y_k^2 x_k \right). \quad (142) \]

In our case the perturbation is \( G(x_n) = (-e^{3x_n^2}/(1 + \mu x_n^2), 0) \). Thus we have

\[ A'(0) = -\frac{e_1}{\omega} \sum_{k = -\infty}^{\infty} \frac{x_{k-1}^2}{1 + \mu x_{k-1}^2} \left[ x_k + \frac{\omega}{2}x_{k-1} + \mu x_k x_{k-1} \right] \]

\[ = \frac{e_1}{\omega} \sum_{k = -\infty}^{\infty} (x_{k+1} + x_{k-1}) x_k^2 \left[ x_{k+1} + \frac{\omega}{2}x_k + \mu x_{k+1} x_k \right] \]

\[ = \frac{e_1}{\omega} \sum_{k = -\infty}^{\infty} \left[ x_{k+1}^2 x_k^2 + \omega x_{k+1}^3 x_k + \mu x_{k+1}^4 x_k + x_{k+1}^4 \right]. \quad (143) \]

We therefore need to calculate sums of the form \( S_1(a, b, \lambda) = \sum_{k = -\infty}^{\infty} \text{sech}^2(\lambda n - a) \text{sech}^2(\lambda n - b). \)

Using the Poisson summation formula we have

\[ S_1(a, b, \lambda) = \sum_{k = -\infty}^{\infty} \int_{-\infty}^{\infty} \exp(2\pi inx) \text{sech}^2(\lambda x - a) \text{sech}^2(\lambda x - b) \, dx. \quad (144) \]
The integral is evaluated using residue calculus:
\[
\int_{-\infty}^{\infty} \exp(\alpha x) \sech^2(\lambda x - a) \sech^2(\lambda x - b) \, dx
\]
\[
= -\frac{\pi}{\lambda} \cosech\left(\frac{2\pi}{2\lambda}\right) \cosech^2 \delta \left[\frac{\alpha}{\lambda} \left(\exp\left[-\frac{xa}{\lambda}\right] + \exp\left[-\frac{xb}{\lambda}\right]\right)\right]
\]
\[+ 2 \coth \delta \left(\exp\left[-\frac{xa}{\lambda}\right] - \exp\left[-\frac{xb}{\lambda}\right]\right),
\]
where \(\delta = a - b\). Setting \(x = -2\pi in\) and performing the remaining sum we get
\[
S_1(a, b, \lambda) = \frac{2\pi}{\lambda} \left[h(\delta) I(a, b, \lambda) + f(\delta) I(a, b, \lambda)\right],
\]
with
\[
I = \phi\left(\frac{\pi b}{\lambda}, \frac{\pi^2}{\lambda}\right) - \phi\left(\frac{\pi a}{\lambda}, \frac{\pi^2}{\lambda}\right) + \frac{\delta}{\pi},
\]
\[
I = -\frac{\partial \phi}{\partial b} - \frac{\partial \phi}{\partial a} - \frac{2}{\pi},
\]
where
\[
\phi(x, u) = \sum_{n=1}^{\infty} \sin(2nu) \cosech(nx) = \frac{K}{\pi} \left[E(am(2Ku/\pi)) - 2uE/\pi\right]
\]
and finally \(h(\delta) = \cosech^2 \delta\) and \(f(\delta) = 2 \cosech \delta \coth \delta\). Similarly, we have
\[
S(a, b, \lambda) = \sum_{k=-\infty}^{\infty} \sech(\lambda n - a) \sech(\lambda n - b) = g(\delta) I(a, b, \lambda),
\]
where \(g(\delta) = \cosech \delta\). The sum \(S_2(a, b, \lambda) = \sum_{k=-\infty}^{\infty} \sech^3(\lambda n - a) \sech(\lambda n - b)\) follows from
\(S_2 = (S - S')/2\), where the primes denote derivatives with respect to \(a\). The sum \(S_3(a, b, \lambda) = \sum_{k=-\infty}^{\infty} \sech^4(\lambda n - a) \sech^2(\lambda n - b)\) can be constructed as \(S_3 = \frac{3}{2}S_1 - \frac{1}{2}S'\) while the last sum \(\sum_{k=-\infty}^{\infty} \sech^4(\lambda n - a)\) is \(S_2(a, a, \lambda)\). Thus we obtain
\[
A'(0) = \frac{e_1}{\omega \mu} \sinh^4 \beta (S_1(t, t - \beta, \beta) - 2 \cosh \beta S_2(t, t - \beta, \beta)
\]
\[+ \sinh^2 \beta S_3(t, t - \beta, \beta) + S_2(t, t, \beta))
\]
which reduces to
\[
A'(0) = -\frac{e_1}{\omega \mu} \sinh^4 \beta \left(4 \coth \beta \left(\frac{K^3 k^2}{\beta^2}\right) dn \left[\frac{2Kt}{\beta} \right] \sn \left[\frac{2Kt}{\beta} \right] \cn \left[\frac{2Kt}{\beta} \right] \right)
\]
\[+ \frac{8K^4 k^2}{3} \left(\frac{2}{\beta^3} \left(2Kt\right)^2 \cn^2 \left[\frac{2Kt}{\beta} \right] - \frac{2}{\beta^3} \left(2Kt\right)^2 \sn^2 \left[\frac{2Kt}{\beta} \right] \right)
\]
\[+ \frac{2K^4 k^2}{3} \left(2Kt\right)^2 \cn^2 \left[\frac{2Kt}{\beta} \right] \sn^2 \left[\frac{2Kt}{\beta} \right] \left[\frac{2Kt}{\beta} \right] \left[\frac{2Kt}{\beta} \right] \),
\]
where $E(k)/K(k) = \pi/\beta$, $K$ and $E$ being the complete elliptic integral of the second kind and the associated complete elliptic integral of the second kind, respectively. Eq. (152) shows that the Melnikov function is a periodic function of $t$ with an infinite number of simple zeros proving the presence of homoclinic chaos in the perturbed map. As a result of the nonintegrability the stable and unstable manifolds of the hyperbolic fixed points of the perturbed map are no longer identical, but intersect and create a homoclinic tangle. Eq. (152) also shows that the separatrix splitting is proportional to the ratio $\gamma/\omega\mu$. The same ratio was found in [83] to limit the parameter region where the map (112) shows regular motion. Finally, from Eq. (152) it is obtained that the distance between successive transversal intersections of the stable and unstable manifolds purely depends on the ratio $K/b$, which in turn only depends on $\omega$ and not directly on the nonlinearity parameters $\gamma$ and $\mu$. The nonlinearity parameters appear only in front of the Melnikov function (153) as a factor regulating the degree of the separatrix splitting. Apparently with higher nonintegrability parameter $\gamma$ the splitting grows whereas the integrability parameter $\mu$ acts in the opposite direction, namely suppresses the splitting.

According to the defining relation between $k$ and $u$ we can obtain that $k$ has a rather slow dependence on $u$ which means that $k$ can be considered small even for rather large $u$ such that it is reasonable consider $k$ as small in Eq. (152). This approximation reduces the complexity of $\Delta t(0)$ considerably. Using small $k$ expansions of the Jacobian Elliptic functions [125]

$$
\Delta t(0) = -\frac{\varepsilon_\gamma}{\mu} A(\omega) \cos\left(\frac{4K}{\beta} t + \theta\right) + \mathcal{O}(k^2),
$$

where

$$
A(\omega) = \frac{2K^3k^2}{\omega\beta^2} \sqrt{\coth^2 \beta + \frac{26K^2}{9\beta^2} \sinh^4 \beta}, \quad \tan \theta = \frac{3\beta \coth \beta}{4K}. 
$$

The distance between successive zeros of the Melnikov function is given by

$$
\Delta t = \frac{\pi \beta}{4K} \approx \frac{1}{2} \ln \left(-\frac{\omega}{2} + \sqrt{\frac{\omega^2}{4} - 1}\right) \equiv \frac{1}{2} \ln(\lambda),
$$

telling us that the distance between two adjacent intersections of the stable and unstable manifold depends solely on the oscillation frequency $\omega$. The distance vanishes at the band edge of $\omega = -2$ and grows logarithmically when $\omega$ ranges further down in the gap. Interestingly, the quantity $\lambda$ in Eq. (155) is identical to the maximal eigenvalue of the linearized map around the hyperbolic point at the origin.

### 3.5. Normal form computation of the homoclinic tangle

In this section we use the Birkhoff normal forms to compute the homoclinic orbit corresponding to the unstable hyperbolic point at the map origin for $\omega < -2$ and $\gamma + 2\mu > 0$. The Birkhoff normal form of an area-preserving map yields a simplified version of the map achieved by a canonical transformation in form of a formal series expansion [126]. Normal forms are powerful tools for analytical determination of homoclinic orbits of two-dimensional maps. Recently Tabacman [127] developed another method for computing homoclinic and heteroclinic orbits relying on
an action principle. In a subsequent section we exploit this method to obtain the orbit heteroclinic to the fixed points \((\hat{x}, \hat{y})\). Later we need the “exact” location of the intersection points of the stable and unstable manifolds to use them as initial data in order to excite stationary localized states of the GDNLS.

We begin by rewriting the map of Eq. (112) as follows:

\[
\mathcal{M} : \begin{cases} 
\tilde{x} = -\omega x - \omega \frac{(y/\omega - \mu) x^2}{1 + \mu x^2} x - y, \\
\tilde{y} = x. 
\end{cases} 
\] (156)

The linear part

\[
\tilde{x} = -\omega x - y, \quad \tilde{y} = x 
\] (157)

is diagonalized through the canonical transformation

\[
P = \lambda^+ x - y, \quad Q = \lambda^- x - y, 
\] (158)

and

\[
\lambda^\pm = \frac{1}{2} \left[ -\omega \pm \sqrt{\omega^2 - 1} \right] 
\] (159)

are the eigenvalues of the linear transformation (157). The inverse transformation is given by

\[
x = \frac{P - Q}{\lambda^+ - \lambda^-}, \quad y = \frac{\lambda^- P - \lambda^+ Q}{\lambda^+ - \lambda^-}. 
\] (160)

After a scaling \(P \rightarrow \sqrt{\mu}P\) and \(Q \rightarrow \sqrt{\mu}Q\) and with the help of \(\lambda \equiv \lambda^+ = 1/\lambda^-\) we obtain for the transformed map:

\[
\bar{P} = \lambda P - \left(\frac{y}{\mu} - \omega\right)\frac{\lambda^4}{(\lambda^2 - 1)^3} (P - Q)^3 \frac{1}{1 + 1/(\lambda - 1/\lambda)^2 (P - Q)^2}, 
\] (161)

\[
\bar{Q} = \frac{1}{\lambda} Q - \left(\frac{y}{\mu} - \omega\right)\frac{\lambda^2}{(\lambda^2 - 1)^3} (P - Q)^3 \frac{1}{1 + 1/(\lambda - 1/\lambda)^2 (P - Q)^2}, 
\] (162)

or its equivalent Taylor expansion about the origin

\[
P = \lambda P + \left(\frac{y}{\mu} - \omega\right) \lambda \sum_{n=1}^{\infty} (-1)^n \left[ \frac{\lambda}{(\lambda^2 - 1)} (P - Q) \right]^{(2n+1)}, 
\] (163)

\[
Q = \frac{1}{\lambda} Q + \left(\frac{y}{\mu} - \omega\right) \frac{1}{\lambda} \sum_{n=1}^{\infty} (-1)^n \left[ \frac{\lambda}{(\lambda^2 - 1)} (P - Q) \right]^{(2n+1)}. 
\] (164)

Birkhoff [126] introduced a canonical transformation based on the series expansion

\[
P = \xi + \sum_{k=2}^{\infty} \sum_{l=0}^{k} p_{kl} \xi^{k-l} \eta^l, 
\] (165)

\[
Q = \eta + \sum_{k=2}^{\infty} \sum_{l=0}^{k} q_{kl} \xi^{k-l} \eta^l, 
\] (166)
such that the \((\xi, \eta)\) map is given by
\[
\xi = U(\xi \eta) \xi, \quad \eta = [U(\xi \eta)]^{-1} \eta.
\] (167)

The function \(U\) depends only on the product \(\xi \eta\) and has a formal series expansion
\[
U(\xi \eta) = \lambda \left( 1 + \sum_{k=1}^{\infty} U_{2k}(\xi \eta)^{k} \right). \tag{169}
\]

Moser \[128\] proved the convergence of the series (167)–(169) in a disc surrounding the origin provided the series in Eqs. (163) and (164) represent analytical functions which is true in our case. Moreover, it was shown, that whenever the inverse map is also analytic, the region of convergence of the series can be extended in narrow strips along the stable and unstable manifolds, respectively \[129\]. Furuya and Ozorio de Almeida \[130\] used the Birkhoff normal form for a precise computation of homoclinic points of the standard map and our approach proceeds along the same lines for the AL-DNLS map.

It is useful to define the auxiliary series
\[
(P - Q)^{2n+1} = \sum_{k=2n+1} \left( d^{2n+1} \right)_{kl} \xi^{k-l} \eta^{l}. \tag{170}
\]

The recursion relations for the expansion coefficients are then determined by
\[
\lambda U_{k-1} \delta_{k,2l+1} - \lambda p_{kl} = \left( \frac{\gamma}{\mu} - \omega \right) \lambda \sum_{n=1}^{(k-1)/2} (-1)^n (d^{2n+1})_{kl} \frac{\lambda}{\lambda^2 - 1} 2n + 1
\]
\[\quad - \lambda^{k-2l} \sum_{n=0}^{p_{k-2n,l-m}(U^{k-2l})_{2n}}, \tag{171}\]
\[
\lambda (U^{-1})_{k-1} \delta_{k,2l+1} - \frac{1}{\lambda} q_{kl} = \left( \frac{\gamma}{\mu} - \omega \right) \frac{1}{\lambda} \sum_{n=1}^{(k-1)/2} (-1)^n (d^{2n+1})_{kl} \frac{\lambda}{\lambda^2 - 1} 2n + 1
\]
\[\quad - \lambda^{k-2l} \sum_{n=0}^{q_{k-2n,l-m}(U^{k-2l})_{2n}}. \tag{172}\]

The stable and unstable manifold of the map \(\mathcal{M}\) are the images of the \(\eta = 0\) and the \(\xi = 0\) axes under the transformation \(U\). Since the Melnikov function possesses infinitely many simple zeros the stable and unstable manifold cross each other in homoclinic points which we can compute from the images of the two axes under \(U\). This method provides the homoclinic orbit with uniform precision. The unstable manifold as the projection on the \(\xi\) axis is determined by the odd-power series
\[
P = \xi + \sum_{k=3}^{\infty} p_{k0} \xi^{k}, \quad Q = \sum_{k=3}^{\infty} q_{k0} \xi^{k}. \tag{173}
for which the coefficients \( p_{k0} \) and \( q_{k0} \) can be given in closed form

\[
p_{k0} = (\gamma - \omega) \frac{1}{\lambda} \frac{1}{\lambda^k - \lambda} \sum_{n=1}^{(k-1)/2} (-1)^n \left( \frac{\lambda}{\lambda^2 - 1} \right)^{2n+1} (d^{2n+1})_{k0}
\]

\[
\approx (\gamma - \omega) \frac{1}{\lambda} \left( \frac{1}{\lambda^k - \lambda} \right) (-1)^{(k-1)/2} \left( \frac{\lambda^2}{\lambda^2 - 1} \right)^k,
\]

(174)

\[
q_{k0} = (\gamma - \omega) \frac{1}{\lambda} \frac{1}{\lambda^k - 1/\lambda} \sum_{n=1}^{(k-1)/2} (-1)^n \left( \frac{\lambda}{\lambda^2 - 1} \right)^{2n+1} (d^{2n+1})_{k0}
\]

\[
\approx (\gamma - \omega) \frac{1}{\lambda} \left( \frac{1}{\lambda^k - 1/\lambda} \right) (-1)^{(k-1)/2} \left( \frac{\lambda^2}{\lambda^2 - 1} \right)^k.
\]

(175)

We have omitted terms of order higher than \( \lambda^{-2} \). Inserting Eqs. (174) and (175) into Eq. (173) we obtain

\[
P = \xi + (\gamma - \omega) \frac{1}{\lambda} \left( \frac{1}{\lambda^k - \lambda} \right) \sum_{n=1}^{\infty} (-1)^n \left( \frac{\lambda^2}{\lambda^2 - 1} \right)^k \left( \frac{\xi}{\lambda} \right)^k.
\]

(176)

If again terms of the order higher than \( \lambda^{-2} \) are dropped the series can be summed up yielding

\[
P = \xi - \left( \frac{\gamma - \omega}{\lambda} \right) \frac{\xi}{1 + (\xi/\lambda)^2} \left( \frac{\xi}{\lambda} \right)^2.
\]

(177)

Correspondingly, we obtain

\[
Q = \left( \frac{\gamma - \omega}{\lambda} \right) \left( \frac{1}{\lambda^k - (1/\lambda)} \right) \sum_{n=1}^{\infty} (-1)^n \left( \frac{\lambda^2}{\lambda^2 - 1} \right)^k \left( \frac{\xi}{\lambda} \right)^k,
\]

(178)

\[
= - \left( \frac{\gamma - \omega}{\lambda} \right) \frac{\xi^3}{\lambda^2} \frac{\xi}{1 + (\xi/\lambda)^2} + \mathcal{O}(\lambda^{-2}).
\]

(179)

Using the inverse transformation of Eq. (160) the unstable manifold is determined by

\[
x = \lambda y \left( 1 + (\gamma - \omega \mu) \left( 1 - \frac{1}{\lambda^2} \right)^3 \frac{y^2}{\lambda^2 + (\lambda^2 - 1)^2 \mu y} \right).
\]

(180)

Apparently there is no intersection for \( \gamma = \omega \mu \) for which the map degenerates to a linear one. Since the map orbits obey the symmetry \( x \leftrightarrow y \) the stable manifold is obtained from Eq. (180) by exchanging \( x \) and \( y \).

### 3.6. Homoclinic, heteroclinic orbits and excitations of localized solutions

We have seen in Section 3.2 that in the map-plane the origin \((x_n, y_n) \equiv (\phi_{n+1}, \phi_n) = (0, 0)\) forms a hyperbolic fixed point \( p \) as long as \(|\omega| > 2\) which possesses its invariant stable and unstable manifolds. Points belonging to the stable manifold \( \mathcal{W}^s(p) \) approach the fixed point \( p \) under map iteration \( \mathcal{M}^n \) for \( n \to \infty \), likewise points on the unstable manifold \( \mathcal{W}^u(p) \) reach the fixed point \( p \) for \( n \to -\infty \). Thus going along the invariant manifolds of the hyperbolic fixed point localized
stationary solutions could be created. However, searching for soliton-like solutions, one has to be aware that the DNLS system is nonintegrable; a fact which normally prevents it from having soliton-like solutions, since these are associated with an integrable system. As already mentioned the integrable Ablowitz–Ladik (AL) equation possesses soliton solutions which are the discrete versions of the solitons of the (integrable) continuum nonlinear Schrödinger equation [16]. These discrete AL-solitons manifest in the integrable map as a perfect separatrix with coinciding stable and unstable manifold. Since the DNLS system is nonintegrable (see Section 3.4) we know that the separatrix is destructed in the sense that the stable and unstable manifolds no longer coincide but rather intersect each other transversally in homoclinic points, creating complicated chaotic dynamics developing eventually Smale horseshoes. The relation between homoclinic and heteroclinic orbits of nonintegrable maps with localized solutions of the underlying lattice system generating the map is known since the pioneering work of Aubry and coworkers [41,42]. Aubry and Le Daeron [42] studied the Frenkel–Kontorova model consisting of an infinite sequence of equal springs and masses under the action of a periodic potential. They interpreted the Frenkel–Kontorova model as a generating variational for the orbits of the standard map and showed that homoclinic (heteroclinic) intersections, called also discommensurations, are attributed to localized states pinned by the lattice. (We refer to the next section for details.) Coste and Peyrard [107] as well as Wan and Soukoulis [82] dealt with the linkage between the homoclinic orbit of the DNLS map and localized states of the lattice. Coste and Peyrard draw the conclusion that “perfect localization in a DNLS system is impossible” because of the residual stochasticity near the hyperbolic points. Instead of exhibiting a “one-peak solution” as in an integrable system where a solution can approach a hyperbolic point as arbitrarily close as is wanted they claim that in a nonintegrable system multipeak solutions are expected to appear. Wan and Soukoulis came to the same conclusion regarding the DNLS system in the context of Holstein’s polaron model. They interpreted the homoclinic chaos with its stochastic behavior of the map orbits in the vicinity of the hyperbolic point as a splitting of the large polaron solution (represented by a soliton-like orbit) into an array of randomly distributed small polarons pinned by the discrete lattice [82].

In contrast to the propositions in [82,107,108], there exist stable stationary localized solutions to the DNLS related to homoclinic and heteroclinic orbits of the related map. This is the case even though there exist neighboring map orbits which are strongly chaotic. The reason is that the localized states rely on the structural stability of orbits homoclinic or heteroclinic to unstable hyperbolic fixed points such that their amplitudes are represented by a homoclinic (heteroclinic) orbit in the corresponding map plane of \( \mathcal{M} \). A homoclinic point \((\phi_n^{h+1}, \phi_n^{h}) \equiv q\) is defined by \( q \in \mathcal{W}^s \cap \mathcal{W}^u \) and \( q \neq p \). Since \( q \) belongs both to the stable and the unstable manifold of \( p \) it follows that \( \mathcal{M}^n(q) \to p \) as \( n \to \pm \infty \).

In order to depict the homoclinic tangle of the global invariant manifolds we approximate the stable respectively the unstable manifold in the vicinity of the hyperbolic fixed point by the linear subspaces (straight lines in the direction of the eigenvectors to the two eigenvalues with modulus apart from the unit circle) of the linearized map. Iterating a few thousands initial points on them several times, we obtain finally the homoclinic tangle of the hyperbolic fixed point. In Fig. 7a we show the homoclinic tangle for the parameter choice of \( \gamma = 1, \omega = 0.883 \) and \( V = 0.2 \). One clearly recognizes the homoclinic points. Points below the symmetry line \( S_0 \) are characterized by \( \phi_{n+1} < \phi_n \) for \( n > 0 \), i.e. belong to \( \mathcal{W}^s \). Each homoclinic point is mapped into another one and after only a few map iterations rapidly approaches the map origin where \( \phi_n \to 0 \).
Correspondingly, the homoclinic points above the line $S_0$ for which $\phi_n < \phi_{n+1}$ for $n > 0$ will be mapped into the map origin in course of the inverse map, i.e. belong to $\mathcal{U}$ reflecting the translational invariance of the discrete lattice under the operation $n \leftrightarrow -n$. 
Let us now use our knowledge about the homoclinic (heteroclinic) orbits to initiate (stationary) localized solutions for the time-dependent DNLS dynamics. In order to invoke the homoclinic map orbit as an initial condition for the dynamics, a sufficiently accurate location of the orbit members (homoclinic intersection points) is demanded. Obviously, the corresponding amplitudes could be read off from the map plane as the coordinates of the homoclinic intersections. However, this may not be accurate enough to ensure that the spatial behavior of the amplitudes of corresponding dynamical trajectory $\psi_n(t) = \phi_n \exp(-i\omega t)$ follows the homoclinic orbit $\phi_n^h$ closely enough, thus representing a nonlinear eigenstate. Therefore we use the normal form of Eqs. (176) and (178) to compute the homoclinic orbit “exactly”.

For a study of the dynamics of soliton-like solutions for the DNLS given in Eq. (44) we use a lattice of chain length $N = 201$. We implement the analytically computed homoclinic orbit $\phi_n^h$ with $n \in \{-N/2, N/2\}$ as initial conditions $\text{Re} \psi_n(t = 0) = \phi_n$ and $\text{Im} \psi_n(t = 0) = 0$. The result for the soliton-like solution is illustrated in Fig. 7b. Using a Fast-Fourier-Transform-routine we determined the oscillation frequency to $\omega = 0.879 \pm 0.004$, which is in fairly good agreement with the value for frequency put in the map, i.e. $\omega = 0.883$. We inserted the (dynamical) amplitudes $|\psi_n(t)|^2$ as diamonds on the map plane in Fig. 7a to show that they coincide with the homoclinic orbit. The stationary localized soliton-like solution has the following amplitude pattern $(\ldots, \dagger, \dagger, \dagger, \ldots)$ where the dots stand for vanishingly small amplitudes. This localized mode is centered at a single site.Aceves et al. showed also that these excitation pattern of DNLS results in stable steady-state solutions [77–79].

In the same manner we proceed with the kink-like (dark soliton) solution for values of $\omega$ inside the linear band. To derive the heteroclinic orbit with high precision we apply a variational approach developed recently by Tabacman [127] to compute homoclinic and heteroclinic orbits for twist maps. The advantage of this method is that it only requires knowledge of the generating function of the map (see Proposition 7 in [127]). The map $D$ can be rewritten in terms of the variables $q_n = \phi_n$ and $p_n = q_n - q_{n-1}$. The corresponding map orbits can be derived from the generating function

$$S(q_n, q_{n+1}) = \frac{1}{2}(q_{n+1} - q_n)^2 + (1/2\mu)(\gamma/\mu - \omega)\ln(1 + \mu q_n^2) - (\gamma/2\mu + 1),$$

with the relations $p_n = -\partial S(q_n, q_{n+1})/\partial q_n$ and $p_{n+1} = \partial S(q_n, q_{n+1})/\partial q_{n+1}$. One can define an action function $W_N$ the critical points of which delivers the orbit heteroclinic to the fixed points at $(q_-, \hat{q}_-; p-, \hat{p}_- = 0)$ and $(q_+, \hat{q}_+; p_+ = 0)$. The action function $W_N$ is then given by

$$W_N(q_0, \ldots, q_N) = \Phi^u(q_0) + \sum_{n=0}^{N} S(q_n, q_{n+1}) - \Phi(q_N),$$

where the functions $\Phi^u(q_0)$ and $\Phi(q_N)$ describe locally the stable and unstable manifolds $\mathcal{W}^u(q_-, \hat{p})$ and $\mathcal{W}^s(q_+, \hat{p})$, respectively. These functions $\Phi^\pm$ can be computed using the linear subspaces at the fixed points. To compute the critical values of the function $W_N$ we used a Newton method. Apparently it is sufficient to obtain one single member of the heteroclinic orbit and then to use the map for getting the others as iterates. When iterating along the stable manifold we approach soon
(typically after 5–8 numbers of iteration) the close vicinity of the hyperbolic fixed points where the orbit stays. Alternatively, one can also use normal form computations in order to generate the heteroclinic orbit. However, for heteroclinic orbits more than one normal form has to be evaluated.

Fig. 8a shows the map plane for the kink-like solution. Again we have inserted the kink amplitudes $|\psi_d(t)|^2$ along the lattice as diamonds in the map plane shown in Fig. 8a.

In this way excitation of the staggered solitons is also possible. Note that staggered localized DNLS modes have been observed experimentally in a real electrical network [23].

The map for the stationary solutions enables one also to predict the existence of another kind of stationary localized solution with amplitude pattern of the form $(\ldots, \uparrow, \uparrow, \uparrow, \uparrow, \ldots)$, i.e. it is supported by a homoclinic orbit having the turnstile as one homoclinic point located on the symmetry line $y = x$, i.e. $\phi_{n+1} = \phi_n$. This localized mode is centered between two lattice sites. Its energy is higher than that of the above mentioned localized mode centered at one single lattice site (see also next section).

We close this section with the remark that the complete dynamical DNLS system is studied in Ref. [132]. It was found that the odd-parity mode is in fact a stable localized standing excitation of DNLS sustaining symmetry breaking perturbations of its mode pattern. Recently Aceves et al. also showed that the preferred stable localized DNLS states are supported by states having exponentially decaying amplitudes around the maximal amplitude at a single-site, i.e. the odd parity mode. On the other hand, the even-parity mode exhibits a dynamical instability and collapses to the odd-parity mode under the impact of symmetry breaking perturbations. These results are in agreement with the findings in [104].

3.7. The soliton pinning energy

As a consequence of the nonintegrability of the map $\mathcal{M}$ and the resulting transversal intersection of the stable and unstable manifolds the soliton-like solutions are pinned, i.e. they cannot be translated over the lattice from one point to an adjacent without overcoming an energetic barrier [118]. The pinning energy can be computed with the help of the normal forms as done in [130] for the solitons of the standard map. We use here another approach based on the findings of the Melnikov function. Kivshar and Campbell [133] studied the pinning energy (Peierls–Nabarro potential barrier) for the localized modes of the DNLS system, i.e. for $\gamma \neq 0$ and $\mu = 0$.

There exist two homoclinic orbits whose points alternate along the invariant manifolds. Each of the homoclinic orbits has one of its points on the symmetry line $S_0$ and $S_1$, respectively. These points rapidly approach the map plane origin under the mapping where they stay most of the time. The homoclinic orbit crossing $S_0$ which we denote by $\{\Phi_{\text{even}}\}$ represents an excitation pattern of $(\ldots, \uparrow, \uparrow, \uparrow, \ldots)$ on the lattice chain. Such a stationary excitation pattern was called even-parity mode in [98] and sometimes also inter-site centered local mode [104]. The other homoclinic orbit $\{\Phi_{\text{odd}}\}$ possesses three large amplitudes $(\phi_-, \phi_0, \phi_1)$ and has the mode pattern $(\ldots, \uparrow, \uparrow, \uparrow, \ldots)$ which was called the odd-parity mode [97] or on-site centered local mode [104]. The point $(\phi_-, \phi_0)$ is located on $S_1$. For positive (negative) $\gamma + 2\mu$ the unstaggered odd-parity (staggered even-parity) mode has lower action (energy) than the unstaggered even-parity (staggered odd-parity) mode. To see this for $\gamma + 2\mu > 0$, one starts iterating the map $\mathcal{M}$ at the turnstile of $x_{\text{even}}^\text{max} = y_{\text{even}}^\text{max}$, (a member of the unstaggered even-parity mode), and goes along the stable manifold in the range of $y > x$ till the next intersection point is met. Then one follows the unstable manifold back to the turnstile. In this
Fig. 8. Soliton-like solutions. (a) The map plane illustrating the heteroclinic connection of the hyperbolic fixed points at \( |\phi_{n+1}| = |\phi_n| = \sqrt{-(\omega + 2V)/\gamma} \). The diamonds represent the squared modulus of the kink amplitudes taken from the dynamics of Fig. 8b. (b) Profile \( |\psi_d(t)|^2 \) of the stationary kink-like solution (dark soliton) of the DNLS. Parameters as in figure (a).

way a closed curve has been described and the area enclosed by it gives the action. We then apply the same procedure for the next pair of homoclinic points. Going down the stable manifold from the largest point of the unstaggered odd-parity mode \((x^\text{max}_{\text{odd}}, y^\text{max}_{\text{odd}})\) one hits the next homoclinic point
and then switches back to the unstable manifold. The obtained closed curve and thus the action (energy) is completely below the first one. Thus only the odd parity map orbit corresponds to a physically relevant discommensuration of lowest energy. In the same manner one can show that for $\gamma < 0$ the staggered even-parity mode has lower action (energy) than the staggered odd-parity one.

Following Aubry [118] we define the pinning energy as

$$E_p = E_{\text{even}} - E_{\text{odd}}.$$  \hfill (181)

The energy functional is given by

$$E(\Phi_n) = \sum_n \left( \frac{1}{2} (\phi_{n+1} - \phi_n)^2 + \frac{1}{2\mu} \left( \frac{\gamma}{\mu} - \omega \right) \ln(1 + \mu \phi_n^2) - \left( \frac{\gamma}{2\mu} + 1 \right) \phi_n^2 \right).  \hfill (182)$$

We can compute $E_p$ “exactly” by using the homoclinic orbits obtained from the normal forms. Moreover, we can exploit the symmetry properties of the map $M$. The Melnikov function provides us with the knowledge of the location of the intersections of the stable and unstable manifolds. Regarding the DNLS term proportional to $\gamma$ as a small perturbation to the AL map, we can get one orbit point for $\{\Phi_{\text{even}}\}$ as the intersection of the AL separatrix with $S_0$ as

$$\phi_{-1}^{\text{even}} = \phi_1^{\text{even}} = \sqrt{-\frac{\omega + 2}{\mu}}.$$  \hfill (183)

To express the symmetry properties of the even parity mode we take the lattice indices $n \in \mathbb{Z} \setminus \{0\}$. Similarly, we obtain for the point $\phi_0$ on $\{\Phi_{\text{odd}}\}$

$$\phi_0^{\text{odd}} = \frac{1}{\sqrt{\mu}} \frac{\omega^2}{4 - 1}.$$  \hfill (184)

The complete homoclinic orbits can be generated with help of the relations

$$\phi_n^{\text{odd}} = \sqrt{\frac{1}{\mu} \frac{\omega^2}{4 - 1}} \sech[2n\mathcal{A}t], \quad n = 0, \pm 1, \ldots,$$  \hfill (185)

$$\phi_n^{\text{even}} = \sqrt{\frac{1}{\mu} \frac{\omega^2}{4 - 1}} \sech[(2n + 1)\mathcal{A}t], \quad n = \pm 2, \ldots.$$  \hfill (186)

Using $\mathcal{A}t$ and $\phi_{\pm 1}^{\text{even}}$ determined by Eqs. (155) and (183), respectively, we obtain

$$\phi_n^{\text{odd}} = \sqrt{\frac{1}{\mu} \frac{(\omega^2 - 4)(\lambda^n + \lambda^{-n})^{-1}}{4 - 1}}, \quad n = 0, \pm 1, \ldots,$$  \hfill (187)

$$\phi_n^{\text{even}} = \sqrt{\frac{1}{\mu} \frac{(\omega^2 - 4)(\lambda^{n/2} + \lambda^{-n/2})^{-1}}{4 - 1}}, \quad |n| > 1.$$  \hfill (188)
Taking the respective excitation patterns into account, we derive for the soliton energies

\[ E_{\text{odd}} = \frac{1}{\mu} \left[ (\omega^2 - 4) \sum_{n=0}^{N} \left( \left( \frac{1}{\lambda^{n+1}} - \frac{1}{\lambda^{-n}} \right)^2 - \left( \frac{\gamma}{\mu} + 2 - \frac{1}{\lambda^{n+1}} + \frac{1}{\lambda^{-n}} \right) \right) \right] + \frac{1}{\mu} \left( \frac{\gamma}{\mu} - \omega \right) \sum_{n=0}^{N} \ln \left( 1 + \left[ (\omega^2 - 4) \frac{1}{\lambda^{n+1}} - \frac{1}{\lambda^{-n}} \right] \right) + O(\lambda^{-2N-2}) \],

(189)

and

\[ E_{\text{even}} = -\frac{1}{\mu} \left[ \sqrt{\omega^2 + 4} \left( \left( \frac{\gamma}{\mu} - \omega \right) \ln(1 + \mu(\phi_{1}^{\text{even}})^2) - \left( \frac{\gamma}{\mu} + 2 \right)(\phi_{1}^{\text{even}})^2 \right) \right] + \frac{1}{\mu} \left[ (\omega^2 - 4) \sum_{n=0}^{2(N+1)} \left( \left( \frac{1}{\lambda^{n+1}/2 + \lambda^{-n+1}/2} - \frac{1}{\lambda^{n/2} + \lambda^{-n/2}} \right)^2 - \left( \frac{\gamma}{\mu} + 2 \right) \frac{1}{\lambda^{n/2} + \lambda^{-n/2}} \right) \right] + \frac{1}{\mu} \left( \frac{\gamma}{\mu} - \omega \right) \sum_{n=0}^{2(N+1)} \ln \left( 1 + \left[ (\omega^2 - 4) \frac{1}{\lambda^{n/2} + \lambda^{-n/2}} \right] \right) + O(\lambda^{-2N-2}). \]

(190)

A plot of the pinning energy as a function of \( \omega \) reveals a remarkable decrease of the pinning energy with increased \( \gamma \) which becomes clear in recalling that the computation of the pinning energy relied on the homoclinic orbit which was identified with location of the zeros of Melnikov function on the unperturbed AL separatrix loop. This computation is the result of a perturbational calculation to first order in \( \varepsilon \gamma \). Moreover, the first correction to Eq. (184) is given by

\[ \phi_{0}^{\text{odd}} = \frac{1}{\gamma} \sqrt{\frac{4\mu^2}{\gamma^2} + (\omega^2 - 4) - 2\mu}, \]

(191)

demonstrating how the maximal amplitude of the odd-parity mode is shifted upwards on the AL separatrix loop with \( \gamma \) diminishing the difference of the peaks of the odd-parity mode and even-parity. Finally the pinning energy decreases with increasing integrability parameter \( \mu \).

We note that we can design an (unstaggered) odd parity mode of desired width by varying \( \omega \). If \( \delta \) denotes a given decrease of the center amplitude then the lattice point \( \tilde{N} \neq 0 \) where \( \phi_{0}^{\text{odd}} \leq \delta \phi_{0}^{\text{odd}} \) holds obeys the relation becomes

\[ \tilde{N} \geq \left[ \frac{2}{\sqrt{\omega^2 - 4 - \omega}} \cosh^{-1}(\delta) \right], \]

(192)

where \([A]\) denotes the integer part of \( A \). Similar expressions can be derived for the staggered odd-parity mode as well as the even-parity modes.

3.8. Summary

We have studied in detail the stationary localized solutions of the GDNLS equation. First, we have described the general properties and features of the GDNLS and shown how this equation...
can be turned into a map by using a stationary solution ansatz. The bifurcational behavior of the fixed points of this map has been set out followed by a discussion how the homoclinic and heteroclinic connections between the unstable fixed points can be related to the bright and dark solitons on the lattice. In Section 3.4 the DNLS term was assumed to be a small nonintegrable perturbation to the integrable AL equation, which allows to calculate the Melnikov function explicitly. The latter describes the splitting of separatrix related to the hyperbolic point at the map origin and leads to the result that the magnitude of the separatrix splitting depends exclusively on the ratio $\gamma/(\omega \mu)$. In investigations [83] this ratio was shown to determine the parameter region where the behavior of the map is regular. Furthermore, the Melnikov function show that the position of the homoclinic intersections along the unperturbed homoclinic orbit solely depends on $\omega$ and not directly on the nonlinearity parameters $\gamma$ and $\mu$. In Section 3.5 the Birkhoff normal forms were applied to calculate the homoclinic orbits related to the hyperbolic point at the map origin. The derived expression was shown to approximate the manifolds with high accuracy.

We have in Section 3.6 discussed how the homoclinic orbit of the related map supports localized solutions to the GDNLS. This means that the irregular behavior of the map through the existence of homoclinic intersections actually ensures the existence of the localized solutions to the GDNLS. We also pointed out, in this way, that the map allows us to design localized excitations patterns of the GDNLS. Designing standing localized solutions of the GDNLS is only possible with the help of the stationary analysis which becomes clear from the fact that the broadness of a localized solution and its spatial exponential decay rate depend barely on the oscillation frequency $\omega$. The latter is accessible only in the stationary equation, whereas the two nonlinearity parameters $\gamma$ and $\mu$ appearing in the time-dependent GDNLS do not play a role for the purpose of soliton designing. Finally, we applied in Section 3.7 the result of the Melnikov computations to calculate the pinning energy of the bright solitons on the lattice and showed that it can be tuned by varying the integrability and nonintegrability parameters, respectively.

It is interesting to compare the current findings with the result of Ref. [131] that continuous wave equations of the type $\Box u = F(u)$ possess time-periodic and spatially localized solutions only for a small restricted class of functions $F(u)$. An example exhibiting time-periodic localized solutions is the completely integrable case of $F(u) = \pm \sin u$. In order to obtain soliton-like solutions of the field equations the authors of [131] used an asymptotic expansion method where the formal solution is represented in an asymptotic expansion as power law of the leading nonlinear term. A base equation containing the essential nonlinearity is derived and the remaining hierarchy of equations is solved by a perturbation theory. The self-localized solution of the base equation is supported by a separatrix loop belonging to a hyperbolic point (the equilibrium state $u = 0$) in the phase plane. It was shown that the dimension of the stable and unstable manifolds $\mathcal{W}^{s,u}$ of the hyperbolic point is, in general, finite. However, for localized solutions of the field system the existence of a separatrix loop with an infinite number of transversal intersections of $\mathcal{W}^{s,u}$ is demanded. Hence the infinite system of intersection conditions is overdetermined which prevents the existence of time-periodic and spatially localized field solutions. Our approach of utilizing the separatrix intersections of a planar map to obtain soliton-like solutions of an infinite lattice systems is successful, since the one-dimensional stable and unstable manifolds on the two-dimensional map plane inevitably intersect transversally as a result of the nonintegrability of the map. In this sense the spatial nonintegrability of the stationary GDNLS with the resulting homoclinic and
heteroclinic tangles has a constructive impact on the excitation of standing solitons on the GDNLS lattice.

4. Effects of nonlinearity in Kronig–Penney models

4.1. Motivation

The Kronig–Penney model [134], introduced more than half a century ago, has remained one of the most popular “theoretical laboratories” in the study of wave propagation in various systems. It has been successfully applied in band structure and electron dynamics studies in ordered solids, localization phenomena in disordered solids and liquids [135], microelectronic devices [136], physical properties of layered superconductors [137] and quark tunneling in one dimensional nuclear models [138].

We review the work on an extension of the well-known (linear) periodic Kronig–Penney model by considering the case where the periodic potential consists of a series of periodically (or more generally, quasiperiodically) spaced delta-functions modulated by the square of the amplitude of the wave function as introduced by Grabowski and Hawrylak in [139,140] and studied also by Coste and Peyrard [107] and Hennig et al. [141,142]. The motivation for studying this model is twofold: On one hand it represents a more realistic, continuous, many-band extension of the “one-band” discrete tight binding model used to study propagation in a periodic nonlinear medium [81,82]. The medium can be thought of as a superlattice, where the width of a layer is much greater than a typical atomic spacing and at the same time much smaller than the layer interspacing. Inside a layer, strong electron-phonon interactions induce polaronic effects which give rise to the nonlinear potential. On the other hand, the model can be used to describe the realistic propagation of electromagnetic (EM) waves through a dielectric superlattice constituted of nonlinear Kerr-type material, where the thickness of the nonlinear layer is much smaller than the layer interspacing.

Under the assumption of a scalar wave approximation, an increase in the amplitude of incident waves has the effect of switching the wave from a “passing” to a “nonpassing” regime; in the latter case the wave is completely reflected. Transmission of information in such a periodically modulated nonlinear transmission line is then possible by using amplitude modulation [141]. In what follows we will use the transfer matrix approach to obtain a Poincaré map that can be casted into a nonlinear difference equation form. We turn the (complex) difference equation into a two-dimensional real map, by making use of the conservation of probability and show numerical results for the transmitted intensity for the “fixed output” problem. We investigate the transmittance for the “fixed input” problem and show how the combined effects of linear instability and homoclinic instability lead to a closing of the forbidden gaps.

4.2. The nonlinear Kronig–Penney model

We consider the stationary problem relating to the transport of a quasiparticle in a one-dimensional nonlinear chain modeled by the stationary nonlinear Schrödinger equation:

\[ E\psi(x) = -\frac{d^2\psi(x)}{dx^2} + \lambda \sum_{n=1}^{N} \delta(x - x_n) |\psi(x)|^2 \psi(x). \]  \hspace{1cm} (193)
Equation (193) defines the nonlinear extension to the Kronig-Penney model (or nonlinear Dirac comb) where $E$ is the energy of possible stationary states, $x$ denotes space and $\lambda$ is a parameter. The periodic potential is taken to be a series of equidistant delta-functions that are additionally modulated by the square of the wave function $\psi(x)$. The locations of the $\delta$-functions $x_n$ are taken on a periodic lattice with unit spacing, i.e. $x_n \equiv n$.

We will focus on two distinct problems: (a) electromagnetic wave propagation in dielectric nonlinear superlattices and (b) transport of quantum mechanical particles, such as ballistic electrons, in nonlinear superlattices. Even though these two problems are quite distinct, they can be treated simultaneously through very similar equations that lead to qualitatively similar results. In particular, it can be shown that for the Kronig-Penney model, the two equations are related by a scaled transformation. For details we refer to Section 4.3. Hence, Eq. (193) with some small changes in notation describes also the propagation of an EM wave in a layered superlattice where the nonlinear slabs (described by the $\delta$-function terms) are much smaller than their spacing [141].

When a wave with momentum $k$ is sent from the left towards the nonlinear chain, it will be scattered into a reflected and transmitted part. On the left of the first $\delta$-function potential encountered by the plane wave we have the incident and reflected waves

$$\psi(x) = R_0 \exp(ikx) + R \exp(-ikx),$$  \hspace{1cm} (194)

and to the right end of the chain the transmitted wave

$$\psi(x) = T \exp(ikx).$$  \hspace{1cm} (195)

We denote with $R_0$, $R$ the amplitudes of the injected and reflected wave at the beginning of the chain and $T$ is the transmitted amplitude at the end of the chain. To study the transmission properties of the nonlinear Dirac comb segment we derive a Poincaré map based on the corresponding (nonlinear) transfer matrix which relates the amplitudes of the wave function on adjacent sides of a single $\delta$-potential. Our approach is similar to the one used for the corresponding linear Kronig-Penney problem [143,144]. Since the nonlinear terms enter only at the locations where the $\delta$-functions are, we can write the general solution of Eq. (193) in the interval $[x_n, x_{n+1}]$:

$$\psi_n(x) = A_n \exp(ik(x-x_n)) + B_n \exp(-ik(x-x_n)),$$  \hspace{1cm} (196)

with $x \in [x_n, x_{n+1}]$ and $A_n$, $B_n$ the amplitudes of the forward and backward propagating waves in the segment $[x_n, x_{n+1}]$, respectively. Employing the boundary conditions at $x = x_n$, i.e. continuity of the wave function and discontinuity of its derivative, we obtain a nonlinear transfer matrix connecting the amplitudes of the transmitted and reflected parts through the single $\delta$-function potential at $x = x_n$:

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \begin{pmatrix} (1 - i\frac{\lambda}{2\pi}) \exp(ik) & -i\frac{\lambda}{2\pi} \exp(-ik) \\ i\frac{\lambda}{2\pi} \exp(ik) & (1 + i\frac{\lambda}{2\pi}) \exp(-ik) \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix}. $$  \hspace{1cm} (197)

The nonlinear nature of our model enters through the modified potential strength $\tilde{\lambda}_n$:

$$\tilde{\lambda}_n = \lambda |A_n \exp(ik) + B_n \exp(-ik)|^2 \equiv \lambda |\phi_n|^2.$$  \hspace{1cm} (198)

Unlike the linear scattering problem, since the amplitude of the wave function enters in each single-site transfer matrix, the total transfer matrix for a chain with $N > 1$ sites cannot be represented as a closed product of the unimodular single-site transfer [36,143–145]. We therefore,
need to iterate the Poincaré map \((A_n, B_n) \rightarrow (A_{n+1}, B_{n+1})\) of Eq. (197) repeatedly for \(n = 1, \ldots, N\). Computations are facilitated if we first transform the matrix relation of Eq. (197) to a difference equation \([143]\). We use the transformation

\[
\begin{pmatrix}
\phi_{n+1} \\
\phi_n
\end{pmatrix} = \begin{pmatrix}
e^{ik} & e^{-ik} \\
1 & 1
\end{pmatrix} \begin{pmatrix}
A_n \\
B_n
\end{pmatrix},
\]

(199)
to go from the “bond variables” \((A_n, B_n)\) to the “node” variables \((\phi_n, \phi_{n+1})\). The combined use of Eqs. (197)–(199) leads to a second order nonlinear difference equation for the node variables \(\phi_n\):

\[
\phi_{n+1} + \phi_n = \left[ 2 \cos(k) + \frac{\lambda \sin(k)}{k} |\phi_n|^2 \right] \phi_n.
\]

(200)

Eq. (200) is formally identical to the stationary discrete nonlinear Schrödinger equation (DNLS) with on-site energy \(E(k) = 2 \cos(k)\), unit transfer matrix element and nonlinearity parameter \(\lambda \sin(k)/k\) \([1]\). In fact there exist a connection between difference equations (tight-binding models) and differential Schrödinger equations \([146,147]\). For example Belissard et al. \([143]\) showed that the Schrödinger equation for a periodic array of delta functions of potentials which can be incommensurate with the lattice of delta functions is equivalent to the Aubry model, that is a difference equation with a quasiperiodic potential \([40]\).

We can utilize the equivalence of Eq. (200) with the DNLS equation of Section 2.1 to reduce the dynamics again to a two dimensional (real-valued) map going along the same lines as described in Section 2.4 to obtain a map \((x_n, z_n) \rightarrow (x_{n-1}, z_{n-1})\) where we study from the beginning the inverse map:

\[
x_{n-1} = \left[ 2 \cos(k) + \frac{\lambda \sin(k)}{2k} (W_n - z_n) \right] (W_n - z_n) - x_n,
\]

(201)

\[
z_{n-1} = \frac{1}{2} \frac{x_n^2 - x_{n-1}^2}{W_n - z_n} - z_n,
\]

(202)

with \(W_n = \sqrt{x_n^2 + z_n^2 + 4J^2}\).

In Fig. 9 we show a number of orbits of the map. The elliptic fixed points of the period-4 island chain are surrounded by (regular) quasiperiodic orbits whereas in the vicinity of the separatrix of the hyperbolic fixed points a thin chaotic layer develops. The evolution of the wave amplitude \(r_n^2\) corresponding to a chaotic orbit in Fig. 9 is illustrated in Fig. 10.

In Fig. 11 we illustrate the transmission behavior of a nonlinear chain with 500 \(\delta\)-potentials in the \(k - |T|^2\) plane. This representation is similar to that used by Delyon et al. and Wan and Soukoulis in the study of the corresponding “one-band” tight binding model \([81,82]\). For a given output plane wave with intensity \(|T|^2\) and momentum \(k\) the mapping of Eqs. (201) and (202) has been iterated. For incoming wave intensities \(|R_0|^2\) that are of the same order of the transmitted intensity the nonlinear chain is said to be transmitting (black area in Fig. 11). A divergent solution, on the other hand, results to absence of transmission (white area in Fig. 11). The curve separating the two different regimes in the \(k - |T|^2\) plane exhibits a rich structure. For momenta \(k = n\pi\)
plateaus appear corresponding to ideal transparency, i.e. $|R_0| = |T|$. Furthermore, above critical intensities $|T|^2$ several branches are created indicating bistable or multistable behavior.

Such multistability is illustrated in Fig. 12 where for $k = 3.1$ and $\lambda = 0.1$ the intensity of the transmitted wave is plotted a function of the incident wave.
Fig. 11. Illustration of the transmission behavior of a nonlinear chain with $N = 200$ and $\lambda = 1$ in the $k - |T|^2$ parameter plane. Transmitting solutions correspond to the dark areas whereas diverging (nontransmitting) solutions are indicated by the white area.

Fig. 12. Transmitted intensity as a function of the incident intensity exhibiting the multistability of the nonlinear transmission dynamics. Parameters $k = 3.1$ and $\lambda = 0.1$ are used.

The curve shows oscillations resulting to numerous different output energies for a given input energy. Multistability in the wave transmission is a genuine nonlinear effect that is not present in the corresponding linear Kronig–Penney model and has been reported in numerous other nonlinear wave transmission studies [81,110,148] (see also Section 2.6).
4.3. Propagation in periodic and quasiperiodic nonlinear superlattices

Novel phenomena such as photonic band gaps and possible light localization occur when electromagnetic (EM) waves propagate in dielectric superlattices [110,149–154]. In an approximation where only the scalar nature of the EM wave is taken into account, wave propagation in a periodic or disordered medium resembles the dynamics of an electron in a crystal lattice. As a result photonic bands and gaps arise in the periodic lattice case whereas EM wave localization is theoretically possible in the disordered case. In the latter case and when the dielectric medium is one dimensional, Anderson-type optical localization has been predicted [149,150]. In an ordered dielectric superlattice, on the other hand, photon band gaps have been demonstrated for various realistic configurations [153]. One issue that has not been widely addressed yet is the possibility of using superlattices with nonlinear dielectric properties and, in particular, the nonlinear Kerr effect, to construct optical devices with desired transmission characteristics [113,150]. Aspects of this problem will be considered here.

Before addressing the actual properties of EM wave propagation in a periodic dielectric with nonlinear properties, let us first derive the stationary equation of EM waves and compare it with that for the electron.

In order to derive the wave equation in a nonconducting medium we start from Maxwell’s equations for the medium and arrive at a wave equation for the electric field \( E \) in the absence of free charges,

\[
\nabla^2 E = \varepsilon \frac{\partial^2 E}{\partial t^2},
\]

where \( \varepsilon, \mu \) are the permittivity and permeability of the medium, respectively. We will write \( \varepsilon \mu = n^2/c^2 \), where \( n \) is the dielectric constant and \( c \) is the speed of light. For more general forms that allow also for a nonlinear response of the medium, we have

\[
n(\omega) = n_0(\omega) + \lambda K |E|^2,
\]

where \( \lambda \) is the wavelength, \( K \) the Kerr coefficient, ranging from \( 10^{-21} \) m/V\(^2\) for helium gas to \( 10^{-7} \) m/V\(^2\) for bentonite in water. Typical glass fiber materials have a value of \( 10^{-16} \) m/V\(^2\) for the Kerr coefficient. In units where \( \mu = c = 1 \), we have

\[
n^2 = (n_0 + \lambda K |E|^2)^2 \approx n_0^2 \left( 1 + \frac{2\lambda K}{n_0} |E|^2 \right) = n_0^2 \left( 1 + \frac{4\pi K}{n_0 k} |E|^2 \right),
\]

where the amplitude of the electric field \( E \) can be \( 10^3–10^6 \) V/m. For plane-wave propagation in the \( z \)-direction we only have to consider the following scalar Helmholtz equation:

\[
\frac{d^2 E(z)}{dz^2} + \frac{n^2(\omega, E(z))\omega^2}{c^2} E(z) = 0,
\]

and in particular consider the inhomogeneous multilayered media where the nonlinear one is much thinner than the linear one. Then for the linear medium, Eq. (204) becomes \( E''(z) + k_1^2 E(z) = 0 \), where \( k_1 = n_1 \omega/c; \) whereas for the nonlinear medium, it becomes

\[
\frac{d^2 E(z)}{dz^2} + k_2^2 \left( 1 + \frac{4\pi K}{k_2^2} |E|^2 \right) E(z) = 0,
\]
where \( k_2 = n_2 \omega / c \). In the context of the Kronig–Penney model with wavenumber \( k = k_1 \), we get

\[
k^2 E(z) = - \frac{d^2 E(z)}{dz^2} + \sum_{n=1}^{N} k^2 \delta(z - z_n)g(E(z))E(z),
\]

(206)

where

\[
g(E(z)) = 1 - \frac{4 \pi x K}{k} |E(z)|^2, \quad \text{and} \quad x = n_2 / n_1.
\]

(207)

Upon comparison with Eq. (205) we note the following similarities and differences: The role of the stationary energy \( E \) of the nonlinear Schrödinger equation of Eq. (205) is played by the wavenumber \( k \) or frequency \( \omega \) in the problem of wave propagation. Furthermore, whereas in the wave case this term \( k \) appears as a factor in the delta-function term, this is not true for the particle case. In fact, it can be shown that Eq. (205) can be transformed into the same form as Eq. (206). In the time-independent case the Maxwell’s equations for EM waves is reduced to the following equation:

\[
- \frac{d^2 \phi(x)}{dx^2} + k^2 \sum_{n} \delta(x - na)g(n)\phi(x) = k^2 \phi(x),
\]

(208)

where \( \phi(x) \) is the complex electric field strength, \( k \) is the wavenumber of the wave and \( g(n) \equiv g(n,|\phi|^2) \) is the term that modifies nonlinearly the \( \delta \)-function strengths. The motion of particles, on the other hand, is describable by the one-dimensional Schrödinger equation:

\[
- \frac{d^2 \psi(x)}{dx^2} + \sum_{n} \delta(x - na)h(n)\psi(x) = E\psi(x),
\]

(209)

where \( \psi(x) \) is the wave amplitude, \( E \) is the energy and \( h(n) \equiv h(n,|\psi|^2) \) modifies the \( \delta \)-function strengths.

Let us define \( z = kx \), and transform Eq. (208) into an equation with respect to the new variable \( z \). Eq. (208) becomes

\[
- \frac{d^2 \phi(z)}{dz^2} + k\sum_{n} \delta(z - nka)g(n)\phi(z) = \phi(z).
\]

(210)

For particles with positive eigenenergy, \( E > 0 \), if we define \( \kappa = \sqrt{E} \), and \( z = \kappa x \), Eq. (209) becomes

\[
- \frac{d^2 \psi(z)}{dz^2} + \frac{1}{\kappa} \sum_{n} \delta(z - n\kappa a)h(n)\psi(z) = \psi(z).
\]

(211)

It is easy to see that Eqs. (210) and (211) will be in the same form, if we define the new \( \delta \)-function strengths \( g(n,\kappa) = kg(n) \) and \( h(n,\kappa) = h(n)/\kappa \), and substitute them into Eqs. (210) and (211), respectively. We note that the Schrödinger representation is more general since the classical wave presentation corresponds only to the \( E > 0 \) solutions of the former.

Due to this equivalence between the one-dimensional particle and classical wave problem, in what follows we will deal primarily with the Schrödinger representation of our problem. But first we will actually compare explicitly the two cases.
4.4. Wave propagation in periodic nonlinear superlattices

4.4.1. Combined linear and nonlinear lattices

We will now consider the case where in addition to the nonlinear \( \delta \)-function there is also a linear term present and thus the potential is of the form \( \sum_{n=1}^{N} \delta(x-n)(1 + \lambda|\psi(x)|^2)\psi(x) \).

Straightforward manipulations similar to the ones used in the standard linear Kronig–Penney problem lead to the following nonlinear difference equation \([141,143,144]\)

\[
\phi_{j+1} + \phi_{j-1} = \left[ 2 \cos(k) + \alpha(1 + \lambda|\phi_j|^2) \frac{\sin(k)}{k} \right] \phi_j,
\]

where \( k \) is the wavenumber associated with the frequency \( \omega(k) = 2 \cos k \). A local transformation to polar coordinates and a subsequent grouping of pairs of adjacent variables \( \phi_{n-1}, \phi_n \) turns Eq. (212) to the following two-dimensional map \([141]\):

\[
\begin{align*}
x_{n+1} &= \left[ 2 \cos(k) + \alpha \left( 1 + \frac{1}{2} \lambda(W_n + z_n) \right) \frac{\sin(k)}{k} \right] (W_n + z_n) - x_n, \\
z_{n+1} &= z_n - \frac{1}{2} \frac{x_n^2 - z_n^2}{W_n + z_n},
\end{align*}
\]

where \( W_n = \sqrt{x_n^2 + z_n^2 + 4J^2}, x_n = 2r_n r_{n-1} \cos(\theta_n - \theta_{n-1}), z_n = r_n^2 - r_{n-1}^2 \) with \( \phi_n = r_n \exp(i \theta_n) \) and \( J \) is the conserved current, i.e. \( J = 2r_n r_{n-1} \sin(\theta_n - \theta_{n-1}) \).

The map \( M \) can contain bounded and diverging orbits. The former ones correspond to transmitting waves whereas the latter correspond to waves with amplitude escaping to infinity and hence do not contribute to wave transmission.

In order to investigate directly the transmission properties of the injected plane waves in the nonlinear dielectric superlattice, we iterate numerically the discrete nonlinear equation of Eq. (212). For the initial condition \([\phi_0, \phi_1] = [1, \exp(i k)]\) we compute the transmitted wave amplitude \( T \) for a superlattice with \( 10^4 \) nonlinear dielectric planes for different nonlinearity parameter \( \lambda \) and wavenumber \( k \). In Fig. 13 we plot the transmission coefficient \( t \equiv |T|^2 \) as a function of the input wavenumber \( k \) for various nonlinearity values \( \lambda \). There are clear transmission gaps whose width (in \( k \)-space) depends on \( \lambda \). We note that with increasing \( \lambda \) the width of each gap increases while in addition more gaps in the range between two gaps develop. This process of gap creating starts in the low energy range and extends with further increased \( \lambda \) also to the high energy region. Finally, above critical \( \lambda \)-values neighboring gaps merge leading to a cancelation of transparency.

In Fig. 14 we plot the injected amplitudes for the linear \( (\lambda = 0) \) and nonlinear \( (\lambda \neq 0) \) cases as a function of the wavenumber \( k \).

We note that the typical linear band gaps (dark areas in Fig. 14a) become exceedingly complicated when nonlinearity becomes non zero (hatched region in Fig. 14b). A region was considered transmitting whenever the transmission coefficient was different from zero. In particular we observe the occurrence of new gaps in previously perfectly transmitting regions. Furthermore, the width of the passing regions (white regions) shrinks with increasing injected wave energy. The diagram was obtained by taking a grid of 500 values of \( k \) and 250 values \(|R_0|\) and iterating Eq. (212) on each individual point of the grid over the \( N = 10^4 \) sites.
Fig. 13. Transmission coefficient as a function of the wave number $k$ for $\lambda$ equal to (a) zero (linear case), (b) 0.2, (c) 1.0 and (d) 4.0. The value of the linear coefficient is $\alpha = 1$ and the amplitude of the injected wave is taken to unity.

The “band structure” shown in Fig. 14 can be obtained directly from the tight-binding-like Eq. (212). In the linear case, i.e. for $\lambda = 0$, the allowed propagating band states are obtained from the well-known Kronig–Penney condition. The second order difference equation for the linear Kronig–Penney problem is

$$
\phi_{n+1} + \phi_{n-1} = \left[ 2 \cos(k) + \frac{\alpha \sin(k)}{k} \right] \phi_n ,
$$

and wave transmission is possible only when

$$
\left| \cos(k) + \frac{1}{2} \frac{\alpha \sin(k)}{k} \right| \leq 1 .
$$

The critical curves in the $\alpha$–$k$ parameter plane separating regions of allowed and forbidden energies, i.e. where the equal sign in Eq. (216) holds, are readily determined as:

$$
k = (2n + 1)\pi ,
$$

$$
\alpha = -2k \cot(k/2) .
$$
Fig. 14. Amplitude of injected wave $R_0$ as a function of the wave number $k$ for $\lambda$ equal to (a) zero (linear case), (b) 1.0. The value of the linear coefficient is $\alpha = 1$. The super lattice has 4000 nonlinear slabs. Transmitting solutions correspond to the hatched area whereas diverging solutions are indicated by the blank area.

and

$$k = 2n\pi,$$  \hspace{2cm} (219)

$$\alpha = 2k \tan(\frac{k}{2}),$$  \hspace{2cm} (220)

where $n = 0, 1, 2, \ldots$ is an integer number. These equations define curves that form the boundaries of ranges of forbidden energies (gap states). The tongues get broader with increasing $\alpha$ and therefore the regions of allowed energies (band states) in between the tongues shrink. But even for large $\alpha$ values the tongues of neighboring gap states do not merge ensuring transparency of the linear chain.

This situation changes drastically in the corresponding nonlinear Kronig–Penney problem. For an appropriate analysis of the wave propagation a nonlinear potential formulation can be invoked.
To this end we exploit the fact that Eq. (212) can be derived by a variational approach $\partial L/\partial \phi_n^* = 0$, where the Lagrangian is given by

$$L = \sum_n (\phi_n^*(\phi_{n+1} + \phi_{n+1}^* \phi_n) - \sum_n \left[ 2 \cos(k) + \alpha \left( 1 + \frac{\sin(k)}{2k} |\phi_n|^2 \right) \right] |\phi_n|^2 . \tag{221}$$

The first kinetic term on the r.h.s. of Eq. (221) is responsible for the transfer along the chain whereas the second term represents the local on-site potentials $U(|\phi_n|)$ which are of Landau–Ginsburg type. These quartic on-site potentials obey radial symmetry and are either convex (for $E = 2 \cos(k) > 0$) or concave (for $E = 2 \cos(k) < 0$). For a discussion of the stability of the wave dynamics evolving in such a potential we first locate the extrema of the potential which follow from $\partial U/\partial |\phi_n| = 0$. In the linear Kronig problem the quadratic potential is

$$U_{\text{lin}}(|\phi_n|) = \left[ 2 \cos(k) + \alpha \frac{\sin(k)}{k} \right] |\phi_n|^2 . \tag{222}$$

There is always a global minimum at

$$|\phi| = 0 . \tag{223}$$

In the nonlinear case, the quartic potential reads as

$$U_{\text{nonlin}}(|\phi_n|) = \left[ 2 \cos(k) + \alpha \left( 1 + \frac{\sin(k)}{2k} |\phi_n|^2 \right) \right] |\phi_n|^2 , \tag{224}$$

and the minimum remains at $|\phi| = 0$. For $k \in [n\pi,(2n + 1)\pi/2)$ the minimum is the global extremum of the potential so that the potential exhibits the same features as in the linear case. In accordance with the condition for linear stability we require analogous to the treatment in Section 2.3 for wave propagation the constraint

$$\left| \cos(k) + \frac{1}{2} \alpha \left( 1 + \frac{\sin(k)}{2k} |\phi|^2 \right) \right| \leq 1 . \tag{225}$$

The instability tongues in the present nonlinear case are broadened indicating stronger parameter instability. This is due to the explicit occurrence of the nonlinearity term on the l.h.s. in Eq. (225) so that the boundaries of the instability tongues in the $k$–$\alpha$ parameter plane become also wave amplitude dependent:

$$k = (2n + 1)\pi , \tag{226}$$

$$\alpha = -2 \cot \left( \frac{k}{2} \right) (1 + \lambda |\phi|^2) , \tag{227}$$

and

$$k = 2n\pi , \tag{228}$$

$$\alpha = 2k \tan \left( \frac{k}{2} \right) (1 + \lambda |\phi|^2) . \tag{229}$$
Due to the fact that in these $k$-intervals wave instability is caused by exceeding an energetic stability border like in the linear case we refer to the corresponding tongues as linear instability tongues.

For $k \in [(2n - 1)\pi/2, n\pi)$ and $\cos(k) < -\pi/2$ a bifurcation appears and the potential has global maxima at

$$|\bar{\phi}_n| = \sqrt{-\left(\frac{2\cos(k)}{\pi} + 1\right)\frac{k}{\lambda \sin(k)}},$$  \hspace{1cm} (230)$$

yielding a set of unstable equilibria. Therefore we have a ring of homoclinic fixed points $\bar{\phi} = R \exp(i\Theta)$ characterized by the radii $|\bar{\phi}|$ and different values of the phase $\Theta \in [0, 2\pi)$. The dynamics of the wave amplitude in the proximity of the homoclinic structure exhibits extreme sensitivity in the choice of the initial momenta $k$ inducing thus “spatial” chaos in the wave transmission. The instability in the proximity separatrix motion manifests itself in a “transient” phase of irregular homoclinic oscillations in the amplitude dynamics. Once the amplitude exceeds the separatrix threshold it blows up to infinity giving rise to a gap state. Due to the nature of the escape process we call the corresponding instability tongues homoclinic instability tongues.

Above critical $|\phi|$-values the linear instability tongues and the corresponding neighboring homoclinic instability tongues merge at $k = (2n + 1)\pi/2$ creating broad forbidden gaps thus leading to impenetrability of the nonlinear chain. This is a purely nonlinear effect that is not present in the linear Kronig–Penney model. In the latter there are always allowed bands however small they might be.

In conclusion one sees that nonlinearity in Kronig–Penney models, arising from strong many-body effects in the electron propagation [155] leads not only to multistability in the transmission of plane waves but also has profound effects on the overall transparency of the chain. While the nonlinear model is not very different from the corresponding linear one in the very small $|\phi|$ regime (respectively $\lambda$ regime), the former exhibits non-transparency for larger $|\phi|$-values: A critical threshold in the values of $|\phi|$ exists above which the lattice becomes opaque to all wave transmission. If we compare the “band structures” of the linear and nonlinear Kronig–Penney models for each wavenumber $k$ and corresponding parameter $\lambda$-values we observe an overall reduction in transmittance in the nonlinear case. Furthermore, we note the appearance of new propagation gaps in the nonlinear case in wavevector regions where there was previously (in the linear case), a transmitting band. This behavior is markedly different from the one reported by Chen and Mills [111] and Kahn et al. [96] in a similar system. The difference, however, lies in the fact that while in the present case we are investigating plane wave propagation, in reference [111] soliton-like motion is studied. The presence of nonlinearity in the latter case assists the solitary wave propagation even at locations inside the gap of the corresponding linear problem. The conclusion reached by comparing these two problems is similar to that obtained in other cases, viz. that in a discrete nonlinear medium wavepackets and modes with bounded support travel more efficiently than plane waves [156].

The presence of nonlinearity in the dielectric superlattice planes alters substantially the transmission properties of the waves. In particular, when the input power $|\phi_0|$ (nonlinear coefficient $\lambda$) is increased new nontransmitting regions appear adjacent to the regular instability regions. Consequently, for a given wavenumber $k$, an appropriate change of the input power of the wave (corresponding to a change in $\lambda$) can switch the wave from a transmitting to a nontransmitting
region. It is then possible by a simple amplitude modulation of the incoming wave to transmit binary information to the other side of the transmission line in the forms of zeros (nontransmitting region) and ones (transmitting region).

4.4.2. Propagation of EM waves

We consider propagation of plane waves in the scalar approximation in a one-dimensional continuous linear dielectric medium. In the medium we embed periodically small dielectric regions that have non-negligible third order nonlinear susceptibility \( \chi^{(3)} \) (Fig. 15). We assume for simplicity that the width of the nonlinear dielectric regions is much smaller than the distance between two adjacent ones. We are thus led to a model for a periodic nonlinear superlattice and the propagation of a plane wave injected on one side of the structure can be described through the a nonlinear Kronig–Penney lattice by the Schrödinger equation:

\[
Eu(z) = -\frac{d^2u(z)}{dz^2} + \alpha \sum_{n=1}^{N} \delta(z - n)(1 + \lambda|u(z)|^2)u(z). \tag{231}
\]

In Eq. (231), \( u \) is the complex amplitude of an incoming plane wave with energy \( E \) along direction \( z \), \( \alpha \) is proportional to the dielectric constant of the dielectric in each superlattice slab and \( \lambda \) is a nonlinear coefficient that incorporates \( \chi^{(3)} \) and the input wave power [157]. The series of equidistant delta-functions represent the effect of the periodic nonlinear dielectric medium on the wave propagation.

We will now show results from the genuine wave case; even though wave propagation is described by a slightly different equation, it actually gives very similar quantitative results. We now consider Eq. (206) and perform the same analysis as previously in the particle case.

In Fig. 16 we summarize the results for transmission in a superlattice with various values of the Kerr coefficients, \( K = 1.19 \times 10^{-9}, 1.19 \times 10^{-8}, 1.19 \times 10^{-7}, 1.19 \times 10^{-4}, 1.19 \times 10^{-3}, 1.19 \times 10^{-2}, \) and 0.119 \( \mu m/V^2 \) for (b)–(h) in the figure, respectively. The lattice size \( N = 377 \) (other values of \( N \) give similar results), lattice constant \( a = 1 \mu m \), and \( \alpha = 0.95 \) in Eq. (207); \( k \) is in the unit of \( \mu m^{-1} \).

Fig. 15. A periodic dielectric superlattice with nonlinear susceptibility due to the Kerr effect. The narrow-striped regions denote the dielectric slabs with nonlinear properties. The periodic value of the nonlinear coefficient \( \lambda \) is approximated by the periodic delta functions.
Fig. 16. Transmission spectrum for different amplitude $E(z)$ for EM waves in alternatingly linear and nonlinear dielectric media. The white regions are transmission regions and the black areas are opaque regions. (a) is the linear case, and (b)–(h) are nonlinear cases with various nonlinear strengths given in the text.
and the field amplitude \( E(z) \) is in the unit of \( \text{V/\mu m} \). We note the qualitative similarity in the transmission properties with the particle case. In addition, we see also a new feature in the “weak” nonlinearity cases. There is a region where nonlinearity reduces the widths of the gaps and in some cases it effectively eliminates them for small \( k \)’s. This means that the transparency of the medium is enhanced in this particular region. We note that for large nonlinearity values the medium becomes opaque for large values of \( k \).

4.5. Transmission in a quasiperiodic lattice-

We review the work on quasiperiodic nonlinear Kronig–Penney models with a sequence of barrier heights as well as sequential intersite distances constructed according to the Fibonacci inflation rule. We find that nonlinearity enhances transparency and reduces the localization properties of the corresponding linear quasiperiodic Kronig–Penney model.

Since the discovery of the quasi-crystalline phase in AlMn exhibiting quasiperiodic properties there has been growing interest in models describing the electron and phonon spectrum of such quasicrystals [158]. Recent advances in nanodevice manufacturing has increased the interest in quasiperiodic one dimensional models [159]. Merlin et al. synthesized the first one dimensional semiconductor superlattice [160]. Quasiperiodic models provide a bridge between the regular ordered lattices of perfect materials and random lattices of amorphous systems. Interest in electronic propagation in quasicrystals has led to a thorough investigation of the band structure of some quasiperiodic systems, such as Penrose tiling and Fibonacci lattices [161–163]. Concerning the localization problem for wave propagation within a linear theory there exist three types of wave functions: localized (normalizable), extended (unnormalizable) and critical. For (electronic) tight-binding models possessing either two types of hopping matrix elements or on-site energy arranged in a Fibonacci sequence one obtains a Cantor-set of allowed energies and the wave function is self-similar and therefore intermediate between a localized and extended state [36,164]. For electron transmission in a one dimensional quasicrystal described by a (linear) Kronig–Penney model with \( \delta \)-potentials heights arranged due to the Fibonacci sequence two kinds of electron energies exist. One correspond to localized states and the other two extended states [165].

Studies on combined effects of nonlinearity and quasiperiodicity on the optical transmission properties of superlattices consisting of nonlinear materials arranged in a Fibonacci sequence were performed in references by Kahn et al. in [166] and Gupta and Ray [167]. Special attention was paid whether the gap solitons which had been found in the corresponding periodic nonlinear lattice exist in the aperiodic case as well. Kahn et al. [166] using a tight-binding like model found no evidence for gap solitons the field envelops turn out to be rather irregular and fast oscillating. Gupta and Ray utilized a nonlinear transfer matrix technique under the assumption of slowly varying envelope functions and established the existence of gap solitons for a choice of the linear optical path in each slab as \( n \pi \) with integer \( n \). But in these parameter ranges the linear transmission is also perfect since it remains unaffected by the quasiperiodicity. Later Johannsson and Riklund studied the electronic transmission properties of a one dimensional deterministic aperiodic nonlinear tight-binding lattice based on the DNLS. Quasiperiodicity in their model enters through arrangements of the on-site energy according to the Thue–Morse sequence [168]. For small nonlinearity the authors found soliton-like solutions in a similar way as in the corresponding periodic model. Contrary to the Fibonacci type aperiodicity the Thue–Morse type aperiodicity
supports transmission in the gaps of the linear regime in the form of gap solitons. With respect to the existence of single-site self-trapped states in aperiodic nonlinear discrete systems Johansson and Riklund concluded from their numerical analysis that there seems to be always self-trapping whenever in the corresponding linear lattice the spectrum is a point spectrum or a singular continuous spectrum. Finally, Hiramoto and Kohmoto extended a linear quasiperiodic tight binding model by adding a Hubbard-type interaction term giving so rise to nonlinearity in the model. They showed that such a term does not affect the Cantor-set character of the spectrum for a Fibonacci model and hence the wave functions stay critical. However for the incommensurate Aubry model the singular continuous character of the spectrum becomes destroyed [163,169].

In the present section we will be addressing the issue of wave propagation in a quasiperiodic superlattice model where the medium has in addition nonlinear properties arising from the optical Kerr effect [113,141,150]. We will study the interplay between nonlinearity and quasiperiodicity and demonstrate that it can be used advantageously in wave propagation in nanodevices. The results obtained are also applicable to problems of electronic propagation in superlattices where the effective nonlinearity stems from many-body interactions [155].

We consider the following general Kronig–Penney equation:

\[
\frac{d^2\psi(z)}{dz^2} + \sum_{a=1}^{N} \lambda_a \delta(z - z_a)g(z)\psi(z) = E\psi(z),
\]  

(232)

where for the linear (L), nonlinear (NL) and the general nonlinear (GNL) models, we define as follows:

\[
g(z) = \begin{cases} 
1, & \text{L} \\
|\psi(z)|^2, & \text{NL} \\
\alpha_0 + \alpha_1|\psi(z)|^2, & \text{GNL}
\end{cases}
\]

where \((\alpha_0, \alpha_1)\) are real numbers.

In Eq. (232), \(\psi(z)\) represents an electronic wavefunction or is the complex amplitude of an incoming plane wave with energy (or frequency) \(E\) along direction \(z\), and \(\lambda_a\) is a coefficient that, in the case of the nonlinear optical medium, incorporates the nonlinear susceptibility \(\chi^{(3)}\) and the input wave power [141,157]. The space-periodic \(\delta\)-functions represent small nonlinear dielectric regions that are periodically embedded in a linear dielectric medium. These nonlinear regions are assumed to be much smaller than the distance between adjacent ones. Quasiperiodicity in this model enters in a twofold way. Firstly, the coefficients \(\lambda_n\) that are assumed to follow the Fibonacci sequence. This sequence follows from the inflation rule: \(S_{l+1} = S_lS_{l-1}\), where \(S_0 = A\) and \(S_1 = AB\). There are only two values of \(\lambda_n\), \(\lambda_A\) and \(\lambda_B\) and the actual value of \(\lambda_n\) at location \(n\) is determined from the Fibonacci rule. We use the following procedure to obtain the sequence [144]:

\[
\mu_{n+1} = [\phi_n + 1/\gamma], \quad \phi_{n+1} = (\phi_n + 1/\gamma) \mod(1),
\]  

(233)

where the rectangular brackets denote the integer part, \(\gamma = (\sqrt{5} + 1)/2\) is the golden mean and we start with \(\phi_0 = 0\) at \(n = 1\). The value of \(\lambda_n\) is \(\lambda_A\) of \(\lambda_B\) when \(\mu_n\) is 1 or 0, respectively.

Secondly, the intersite distances \(d_n = z_n - z_{n-1}\) are assumed to be quasiperiodic and follow the Fibonacci sequence. There are two values of \(d_n\), \(d_n = 1\) or \(d_n = a > 1\) resulting from the actual
location of $z_n$ which is determined by the rule

$$z_n = n + (a - 1) \left[ \frac{n + 1}{\omega} \right]$$

with $\omega = (1 + \sqrt{5})/2$ being the golden mean and the bracket $[\cdot]$ denoting the integer part. When the intersite distance $d_n$ is a constant, it can be shown that finding the solution of Eq. (232) is equivalent to solving the problem of a nonlinear tight-binding model [143,144]; but this is no longer true for the quasiperiodic nonlinear lattices which are being studied here.

We investigate the scattering problem of a quasiparticle with momentum $k$. The first study deals with the NL-case when quasiperiodicity enters through an arrangement of the heights of the delta-barriers due to the Fibonacci sequence while the distances between them is kept constant. Plane waves are sent from the left towards the nonlinear chain and will be scattered into a reflected and transmitted part.

Straightforward manipulations similar to the ones used in the standard linear Kronig–Penney problem lead to the following nonlinear difference equation for $t_n$, (234)

$$t_{n+1} + t_{n-1} = \left[ 2 \cos(k) + \lambda_n |\psi_n|^2 \sin(k) \right] t_n,$$

where $k$ is the wavenumber associated with the energy (or frequency) $E(k) = 2 \cos(k)$. Eq. (234) can be treated as a nonlinear map for various initial conditions corresponding to waves injected initially from the left and propagating towards the right side of the chain.

In Fig. 17 we illustrate the transmission behavior in the $|R_0| - k$ parameter plane for the linear Fibonacci Kronig–Penney model (Fig. 17a) and the nonlinear one (Fig. 17b). Dark regions represent gaps in the wave propagation whereas the passing regions are white. In the linear case, i.e. when the term $|\psi_n|^2$ is absent from Eq. (234), we have the typical band structure resulting from quasiperiodicity [36]. We note that the effect of nonlinearity alters substantially this structure resulting in enhanced propagation for small initial intensities. The lattice is transparent for essentially all wavenumbers $k$ at low intensities. In particular, the dominant linear gap for $k$-values approximately less than $k \approx 2$ is reduced drastically. In the higher intensity region, on the other hand, the forbidden lines seem to coalesce together to form well defined nonlinear gaps that are interrupted periodically from propagating resonance-like zones. The latter occur for $k$-values that are multiples of $\pi$; for these wavenumbers the nonlinear term is effectively canceled leading to perfect propagation.

The nonlinear lattice model we presented here has applications in the propagation of electrons in superlattices and electromagnetic waves in the dielectric materials. In the latter case a quasiperiodic linear term should also be included in Eq. (232) representing the linear dielectric constant of the material. The modification in the results due to this term will be studied below in the context of the GNL model.

4.6. Transmission in a quasiperiodic lattice-II

In the previous section, we have studied a lattice with spatially periodic potentials whose bivalued strengths are arranged in a quasiperiodic sequence [141]. It turned out that while
Fig. 17. Injected wave intensity as a function of the wave number \( k \) for a Fibonacci chain of length \( N = 10^4 \). (a) Linear quasiperiodic Kronig–Penney model and (b) nonlinear model. The values of the coefficients \( \lambda_n = \pm 1 \) in both cases and are distributed according to the Fibonacci sequence. The dark areas denote gaps or nonpropagating regions.

quasiperiodicity destroys the transparency of a linear superlattice for small wave numbers (long waves), nonlinearity enhances it in a self-trapped mechanism. We study the Kronig–Penney model here with the sequential intersite distance being quasiperiodic [170]. We will consider mainly the electronic wave for positive potentials but will discuss the results for negative (attractive) potentials, and compare them with the transmission of electromagnetic waves. Finally, we will explain the enhancement of transparency of the quasiperiodic chain for low intensity long waves.

We will discuss the propagation of plane waves and the algorithm for numerical calculations in Section 4.6.1; we will also analyze and compare the transmission properties of the linear and nonlinear models and investigate phase correlations in Section 4.6.2. Section 4.6.3 is devoted to the analysis of long wavelength waves and their transmission at low intensity.
4.6.1. Transmission of plane waves

In the interval between \( z_n \) and \( z_{n+1} \) the solution of the Schrödinger equation can be written as

\[
\psi_n(z) = A_n e^{ik(z-z_n)} + B_n e^{-ik(z-z_n)}
\]

where \( k \) is the wave vector.

We want to establish a nonlinear transformation, connecting the amplitudes \((A_n, B_n)\) and \((A_{n-1}, B_{n-1})\) on adjacent sides of the \( \delta \)-function potential, such that

\[
\begin{pmatrix}
A_n \\
B_n
\end{pmatrix}
= P_n
\begin{pmatrix}
A_{n-1} \\
B_{n-1}
\end{pmatrix},
\]

(235)

where \( P_n \) is the symbolic nonlinear operator, or a nonlinear map which projects one set of complex numbers to another. The transformation in Eq. (235) is generally non-symplectic, although the transformations on \((\psi_n, \psi'_n)\) are. This is because unlike \((\psi_n, \psi'_n)\), \((A_n, B_n)\) are not canonical variables. Similarly, as in the linear Kronig–Penney problem, straightforward manipulations considering the continuity of the wave functions and discontinuity of their derivatives at the boundary near the potential, lead to a (nonlinear) Poincaré map for \( A_n \) and \( B_n \). In order to simplify notations we define first for the amplitudes

\[
\begin{pmatrix}
\bar{A}_{n-1} \\
\bar{B}_{n-1}
\end{pmatrix}
= (A_{n-1} e^{ikd_n})
\]

\[
= (A_{n-1} e^{ikd_n})
\]

where \( d_n = z_n - z_{n-1} \) is the distance between two consecutive potentials. We obtain the following Poincaré map for the nonlinear model:

\[
\begin{pmatrix}
A_n \\
B_n
\end{pmatrix}
= P_n
\begin{pmatrix}
A_{n-1} \\
B_{n-1}
\end{pmatrix}
= \left( \bar{A}_{n-1} - i(\lambda/2k)|\bar{A}_{n-1}|^2(\bar{A}_{n-1} + \bar{B}_{n-1}) \right)
\]

\[
= \left( \bar{B}_{n-1} + i(\lambda/2k)|\bar{A}_{n-1}|^2(\bar{A}_{n-1} + \bar{B}_{n-1}) \right)
\]

and for the inverse transformation, we have the following:

\[
\begin{pmatrix}
A_{n-1} \\
B_{n-1}
\end{pmatrix}
= P_{n-1}^{-1}
\begin{pmatrix}
A_n \\
B_n
\end{pmatrix}
= \left( [A_n + i(\lambda/2k)|A_n + B_n|^2(A_n + B_n)]e^{-i(kd_n)} \right)
\]

\[
= \left( [B_n - i(\lambda/2k)|A_n + B_n|^2(A_n + B_n)]e^{i(kd_n)} \right).
\]

For a finite chain of \( N \) sites, the final coefficients of the wave function is:

\[
\begin{pmatrix}
A_N \\
B_N
\end{pmatrix}
= \prod_{n=N}^{1} P_n
\begin{pmatrix}
A_0 \\
B_0
\end{pmatrix}
\]

(236)

Eq. (236) is a nonlinear map; for various initial conditions it describes waves injected initially from the left, and propagate towards the right side of the chain. Therefore, Eq. (236) or its inverse form can be used to study the transmission properties of the lattice by assuming a given pair of either \((A_0, B_0)\) or \((A_n, B_n)\). The results are analyzed in order to obtain the transmission properties of the lattice.

In Fig. 18, we show the transmission behavior in the \(|R_0| - k\) parameter plane, where \(|R_0|\) is the amplitude of the injected wave for the linear Kronig–Penney Fibonacci (Fig. 18a), the nonlinear (Fig. 18b), and the GNL models (Fig. 18c). Dark regions represent gaps in the wave propagation whereas the passing regions are white. Comparing with the periodic case, Fig. 18 has more structure in the spectrum of the quasiperiodic lattice than the spectrum for a periodic structure shown in Fig. 14. We note that the effect of nonlinearity alters substantially this structure resulting...
in enhanced propagation for small initial intensities. The lattice is transparent for essentially all wavenumbers \( k \) at low intensities. In particular, the dominant linear gap for \( k \)-values approximately less than \( k = 2 \) is reduced drastically. The boundary between the gap and the transmission regions for small \( k \) is almost linear due to the self-trapping effect of the nonlinear medium for the long wave (Section 4.6.3). In the higher intensity region, on the other hand, the forbidden lines seem to coalesce together to form well defined nonlinear gaps that are interrupted periodically from propagating resonance-like zones. The latter occur for \( k \)-values that are multiples of \( \pi \); for these wavenumbers the nonlinear term is effectively canceled leading to perfect propagation. For the
GNL model, the results depend on the choice of $a$'s. We find that, when $a_1 < 0$, the transparency is enhanced as compared with the corresponding linear case; otherwise, it is reduced.

To analyze further the effects of nonlinearity in the model we calculate the transmission function $t = |T|^2/|R_0|^2$, where $T$ is the transmitted amplitude in the end of the chain and $R_0 = |\psi_0|$, is the incident wave amplitude at the beginning of the chain.

In Fig. 19 we plot the transmission function vs. wavenumber $k$ with incident wave amplitude $R_0 = 0.2$. As expected, the linear case shows (Fig. 19a) that the transmission or gap does not depend on the amplitude, and a large gap area exists for small $k$; the nonlinear model (Fig. 19b) demonstrates almost a total transparency for the entire spectrum of $k$, because the dependence of the interaction between the wave and the medium on the wave amplitude makes it easier for waves with relatively small amplitudes to transmit. The picture becomes more complicated when both linear and nonlinear interactions are included. An example is given in Fig. 19c.

In Fig. 20, we plot transmission as a function of the chain length $N$ for the linear Fibonacci Kronig–Penney case (a) and the nonlinear ones ((b) and (c)) for $k = 0.2350$. In the linear case transmission coefficient $t$ drops exponentially with $N$, whereas in the nonlinear and general nonlinear cases the transmission remains a constant, and we have windows with perfect transmittivity in (b). Fractal structure is present for both linear and nonlinear lattices due to the quasiperiodicity of the lattices. In Fig. 22, the boundary separating transmitting (white) from non-transmitting (grey) regions also shows a fractal structure, specially at large $k$-values. Similar fractal behavior has been reported by Delyon et al. for a related model [81].

4.6.2. Correlation functions

The enhancement in coherence resulting from the nonlinear term can be seen also in the correlation function. We go to polar coordinates $\psi_m = r_m \exp(i\theta_m)$ and define the phase correlation
Fig. 19. Transmission vs. wavenumber for linear and nonlinear Fibonacci chains. The initial wave amplitude is 0.2 and the length of the Fibonacci chain \( N = 987 \). (a) The linear Kronig–Penney model. (b) The nonlinear model. It shows that transmission is enhanced for almost the whole spectrum of \( k \) at low intensity. (c) The GNL model with \( x_0 = x_1 = 0.5 \). It shows a mixed result for transmissions. But for small wavelength, transmission in general is reduced as compared with the corresponding linear model.
function $C(m)$ as

$$C(m) = \langle \theta_{m+1} \theta_m \rangle = \frac{1}{N} \sum_{n=1}^{N} \theta_n \theta_{n+m},$$

(237)

where $m$ is a lattice site. In Fig. 21 it can be easily seen that for the linear Fibonacci lattice, $C(m)$ drops almost linearly as a function of $m$ (Fig. 21a), in contrast with the well-known exponential decay of correlation functions in a random lattice. For the nonlinear Fibonacci lattice shown in Fig. 21b, however, the correlation functions are well maintained in amplitudes for $m$ up to $10^4$. For the general nonlinear case with $\alpha_0 = \alpha_1 = 0.5$, (shown in Fig. 21c), correlation in wavefunctions is also substantially enhanced comparing to the linear case, but not as strong as in the pure nonlinear case.

4.6.3. Low-intensity transparency for long waves

In this section we will use the long-wavelength approximation and show in details why transparency is enhanced for low-intensity waves. With long waves, $kd_n \ll 1$, $\exp(\pm ikd_n) \approx 1 \pm ikd_n$. We will be able to solve the nonlinear equations in Section 4.6.1 by taking the long-wave approximation. Let us define

$$\psi_n \equiv \psi_n(z_n) = A_n + B_n,$$

(238)

$$\zeta_n = B_n - A_n.$$

(239)

According to Eq. (236), $\psi_n$ is the wavefunction at site $n$, whereas $\zeta_n$ is only a temporary variable for algebraic convenience. Then Eqs. (238) and (239) can be expanded and regrouped to form $\psi_n$ and
Fig. 21. Phase correlation functions $C(m)$ of propagating waves for three different quasiperiodic K–P models; (a) the linear lattice, (b) nonlinear lattice, and (c) the GNL lattice. In the linear case, the amplitude of $C(m)$ decays almost linearly with $m$; in the nonlinear case, $C(m)$ does not decay up to $m = 10000$; in the GNL case, $C(m)$ drops more slowly than the linear case. Notice different scales are used for (a)–(c).

$\xi_n$, and by keeping only the first order terms, it is easy to see that

$$
\begin{align*}
\psi_n &= \psi_{n-1} - ikd_n\xi_{n-1}, \\
\xi_n &= \xi_{n-1} - ikd_n\psi_n + i\frac{\lambda}{k}|\psi_n|^2\psi_n.
\end{align*}
$$

(240)

Taking the continuum limit as $k \to 0$, or more appropriately, $k^{-1} \gg d_n$, Eq. (240) becomes a pair of coupled differential equations:

$$
\frac{d\psi(n)}{dn} = -ik\xi(n), \quad \frac{d\xi(n)}{dn} = -ik\psi(n) + i\frac{\lambda}{kd}|\psi(n)|^2\psi(n),
$$

(241)
where we have replaced $d_n$ with its average $d$. Substituting the second equation into the first one in Eq. (241) after differentiation, we obtain the following second order differential wave equation:

$$
\dot{\psi}(n) = -k^2\psi(n) + \frac{\lambda}{d}|\psi(n)|^2\psi(n) .
$$

(242)

We can distinguish three cases.

The linear case. Replacing $|\psi|^2$ with 1 in Eq. (242) yields the linear equation:

$$
\ddot{\psi} = -\left(k^2 - \frac{\lambda}{d}\right)\psi = -\sigma^2\psi .
$$

When $\sigma^2 < 0$, wavenumber $k$ is small, there are only exponential solutions, which results in localized state. Roughly speaking, extended states will happen when $k$ is in the order of $k_c \equiv \sqrt{\lambda/d}$. For example, in the previous section, we used $\lambda = 1, d = 1.618$, so that $k_c = 0.786$, and this result is consistent with Fig. 19a.

The nonlinear case. Let $\psi(n) = \psi_0 \exp[i\sigma n]$ be a solution of Eq. (242), then we find

$$
\sigma^2 = k^2 - \frac{\lambda}{d}|\psi_0|^2 .
$$

(243)

Unlike the linear case, whether $\sigma$ is real or imaginary now depends on the intensity of the wave $|\psi_0|$. As long as $|\psi_0| < \sqrt{\lambda/d} k$, there will be propagating waves and hence extended states. Let $\sigma = 0$, we have

$$
|\psi_0| = \sqrt{\lambda/d} k .
$$

(244)

Eq. (244) represents the boundary that separates the gap state from the propagating state for very small $k$. Fig. 22 shows the result from numerical calculation which agrees with Eq. (244) for small $k$. We used $\lambda = 1$, and the average intersite distance $d = 1.618$.

The general nonlinear case. Similarly, for the GNL model, the low-intensity wave equation becomes:

$$
\ddot{\psi} = -\left(k^2 - \frac{\lambda}{d}(\alpha_0 + \alpha_1|\psi|^2)\right)\psi .
$$

For solution of the type of $\psi(n) = \psi_0 \exp[i\sigma n]$, we find

$$
\sigma^2 = k^2 - \alpha_0\frac{\lambda}{d} - \alpha_1|\psi_0|^2 .
$$

Generally, transmission would be more difficult for small $k$ because of the presence of the linear term, and it will get worse if $\alpha_1 > 0$. Compared with the corresponding linear model, better transmission would be achieved for small wavenumber $k$, if the nonlinear term dominates over the linear term, $\alpha_1 \gg \alpha_0$.

The main result that we have shown in the last two sections is the enhancement of transmissions at low wave intensities from a spatially quasiperiodic Kronig–Penney model, in which nonlinearity is added through doped layers in the case of electronic transport in a semiconductor superlattice, or Kerr-type nonlinear media in the case of light transmission. Nonlinearity in the form contained in
Eq. (232) is shown to assist the waves in defying the quasi-random properties of the medium. This effect seems also to be present in genuine nonlinear and disorder segments but with some differences [156]. The nonlinear lattice model we presented here has applications, as pointed before, in the propagation of electrons in superlattices and electromagnetic waves in the dielectric materials. Although we have shown here explicitly only the results for positive potentials ($\lambda > 0$ in Eq. (232)), it is worthwhile to mention that similar results about the enhancement of transmission by nonlinearity exist for negative potentials ($\lambda < 0$) as well.

4.7. Field dependence and multistability

Over the last several decades there has been a continuous interest in the study of electrical field-induced effects in crystals or other periodic structures. There are fundamental mathematical difficulties owing to the destruction of translational symmetry and the pathological effect of divergence for an infinite lattice in the presence of an external field that still prevent the finding of a complete solution for this problem [171]. In this chapter, we study electrical field-induced transport phenomena of ballistic electrons in a finite semiconductor superlattice. We will study first linear effects induced by an external field and subsequently we will see how these effects get modified by nonlinearity. We will use the Kronig–Penney model in both linear and nonlinear cases and solve the Schrödinger equation without the approximations of weak field or weak interwell couplings. In Section 4.7.1, we will study the field-induced changes in transmission spectrum and the interplay between the Wannier–Stark localization and the field-induced inter-subband tunneling for the linear effects [172]. In Section 4.7.6, we will introduce the self-consistent potentials and study the nonlinear space-charge effects in a doped semiconductor superlattice, and explain the experimentally observed multistability and discontinuity of electroconductance [173].
4.7.1. Electric field-induced changes in the transmission spectrum of electrons in a superlattice

In this section, we study the transmission problem of ballistic electrons in a finite superlattice of rectangular barriers in the presence of a homogeneous electric field. A total transfer matrix is constructed, based on the eigenfunctions of the field-dependent Hamiltonian. An explicit solution is given for the transmission probability $T$ for a lattice of $\delta$-function potentials. Numerical results show that, with increasing field strength, transitions occur in $T$ at fixed energy, from transmission to gap and back to transmission. In addition to shifts of band edges to lower energies, almost complete disappearance of lower transmission bands occurs for large fields. We also discuss the connections of our findings with experimental results, especially the electro-optical effects.

4.7.2. The Wannier–Stark localization

The energy spectrum and transmission property of an infinite crystal in the presence of a constant electric field was first studied by Wannier [174], and the Wannier–Stark (WS) ladder effect and Bloch oscillations has been discussed and debated over the years [175–178]. The predicted effect was made for the one-band tight-binding model or a system that resembles such a model, in which the energy levels of the crystal should contain ladder-like structures. For a lattice with a periodic potential of period $a$, it can be easily shown that an electron restricted to a single energy band of width $\Delta$, and without the presence of any scattering, will demonstrate an oscillation in both real and reciprocal spaces [179]. It is easy to see that the period of Bloch oscillation is just $\omega_B = e\phi/a/\hbar$, and the spatial extension of the electron is $L = \Delta/e\phi$, where $\phi$ is the strength of the electric field.

However, for almost three decades, WS ladder and Bloch oscillation had eluded experimental observations until the mid-1980s. It has been argued as early as the 1970s, the WS localization could be easier to be found in a semiconductor superlattice than crystals [180]. This is because in the superlattice, the lattice constant (10–100 Å) is comparable with the electronic wavelengths; therefore, the quantum-mechanical interference effects, which are partly responsible for the formation of WS ladders, are more important in a superlattice than in the crystals. Wannier–Stark localization has been experimentally observed through optical emission and absorption experiments in semiconductor superlattices of GaAs/Al$_x$Ga$_{1-x}$As [181–183], formed by alternating thin layers of GaAs and GaAlAs. Considerable theoretical work has also been done [184,185]. In the GaAs/GaAlAs system, for a certain range of field, the heavy-hole states are fully localized whereas the electron states are still partially extended. Interband optical transitions between electron and hole states could give rise to well-defined absorption or emission spectra with the following characteristics [186]: (1) The spectral lines would be equidistant in energy, the separation being the Stark energy $\Delta E = h\omega_B$. (2) The energy of the central line would be independent of the field to the first order, but its strength would increase with increasing field. (3) The energies of the central lines of the upper branches (relative to the central line) of the spectrum would increase linearly with field at the rate of $n\omega_B$ ($n = 1, 2, 3, \ldots$), where $n$ represents the neighbor index with respect to the central line. The lines of the lower branch would decrease similarly with increasing field.

In dealing with bulk solid state problems, semiclassical treatments of electrons in transport problem are often utilized, but such methods are not valid for mesoscopic systems such as quantum wires and superlattices in which the electron's de Broglie wavelength is comparable with the system's spatial parameters. In dealing with quantum well problems in the presence of an electric field, we notice that the following considerations can significantly affect the results: (a) whether one
Fig. 23. Schematic diagram of a quasi-one-dimensional semiconductor superlattice consisting of two different kinds of materials (upper part), and the electric field-induced structural changes in the square-well/square-barrier potentials $V_0$ (lower part).
mechanical wave coherence and interferences will be maintained when the mean free paths of electrons are much larger than the superlattice constant (interval between two neighboring unit cells). Electrons experience a potential barrier and are consequently scattered at each interface between two layers. In other words, we consider a model of periodic rectangular wells. When an external electric field is applied to the superlattice, the potential wells become tilted, and each site has a potential energy different from its neighbors. Here we will solve the problem exactly, without treating the electric field as a weak field or discretizing the potentials modified by the field. The formal solution shows that the gap regions are shifted toward lower energy and become wider under increasing field. In particular, we find that a region of the transmission spectrum undergoes a transition from transmission to gap and back to a transmission state, with stronger fields. We will illustrate how a gap state can be gradually brought into an extended state under the influence of the field and vice versa.

The one-dimensional Schrödinger equation of a single electron with energy \( E > 0 \) moving in a quantum dot superlattice of \( N \) periodic blocking potentials \( \psi(x) \), is

\[
-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \sum_{n=1}^{N} V(x - x_n) - e\mathcal{E}x \psi(x) = E\psi(x),
\]

where \( V(x - x_n) \) is the potential at site \( n \), \( V(x - x_n) = 0 \) except for the intervals \( x_n < x < x_n + b \), where it equals \( V_0 \); \( x_n = na \), where \( a \) is the lattice constant, and \( b \) is the well width.

Fig. 24 shows the influences of the periodic potential barriers on the transmission of the electrons. The transmission spectra as a function of \( ka \) for 20 different lattice sizes \( N \) are plotted in a quasi three-dimensional diagram for comparison, where \( k = \sqrt{2mE/\hbar^2} \), and \( a \) is the lattice constant. The first gap \( (ka < 0.6) \) exists regardless of the size of the lattice, which corresponds to a minimum energy requirement for transmission. However, when the lattice size \( N \) is small, the Bragg’s backscattering effect is not strong enough to produce the second and third gaps in the transmission spectra; but even for small \( N \), we can still see that transmission is reduced at the locations where Bragg’s condition, \( ka = n\pi \) (\( n \) is integer) is nearly satisfied. In Fig. 24, we use the following parameters: lattice constant \( a = 20 \, \text{Å} \), barrier strength \( V_0 = 0.25 \, \text{eV} \, \text{Å} \), and the electric field \( \mathcal{E} = 0 \). For each of the 20 spectrum curves in Fig. 24, the range of transmission coefficient is from 0 to 1.

Before we look for the solutions, we notice that in the presence of the electric field, plane waves are not eigenfunctions of Eq. (1), nor is wavenumber \( k \) a good quantum number in this problem. Nevertheless, if the electric field is relatively weak, one can still use plane waves and treat \( k \) as a semiclassical quantity, which changes by a discrete amount from site to site; band shifts are expected owing to the lifted energy levels of the left-hand side of the lattice relative to the right-hand side. However, when the field is larger, a full quantum-mechanical approach is needed to reveal the electronic transport behavior, and we now proceed to give that solution. If we define a characteristic length \( l(\mathcal{E}) = (h^2/2m e\mathcal{E})^{1/3} \), and a dimensionless parameter \( \lambda(\mathcal{E}, U) = (2m/\hbar^2 e^2 \mathcal{E}^2)^{1/3} U \), where \( U = E \), or \( (E - V_0) \), for first and second media, respectively, then, it can be shown that inside each layer, Eq. (1) can be transformed into a Bessel Equation of order (1/3) (see Ref. [189] for the transformation), and the solutions for propagating waves can be expressed as a combination of Hankel functions of the first and second kinds (or equivalently as Airy functions). The forward and backward propagating waves between \( x_{n-1} \) and \( x_n \) consequently are combined to
give the following solution:

\[ \psi^{(i)}_n(z) = A^{(i)}_n z^{1/3} H^{(1)}_{1/3}(z) + B^{(i)}_n z^{1/3} H^{(2)}_{1/3}(z) , \tag{246} \]

where \( i = 1, 2 \) indicating the first and second medium respectively, and

\[ z(x, \varepsilon, U) = \frac{2}{3}(\lambda(\varepsilon, U) + x/l(\varepsilon))^{3/2} \]

is the new dimensionless coordinate; \( (A^{(i)}_n, B^{(i)}_n) \) are amplitude constants, which will be determined solely by boundary conditions; and \( H^{(1,2)}_{1/3}(z) \) are the Hankel functions of the first and second kind, respectively.

By differentiating Eq. (246) and using the recurrence relation of Bessel functions,

\[ \frac{d}{dz}(z^v J_v(z)) = z^v J_{v-1}(z) , \]
where $J_\ell(z)$ is any kind of Bessel function, we obtain $d\psi/dx$ as follows:

$$\frac{d\psi_n^{(i)}}{dx} = \frac{1}{k_0} (\xi z)^{\frac{\ell}{2}} \left[ A_n^{(i)} H_n^{(1)}(\xi z) + B_n^{(i)} H_n^{(2)}(\xi z) \right].$$  \tag{247}

Considering the continuity of $\psi(x_0)$ and $d\psi/dx$ at the interfaces of different layers, a transfer matrix between consecutive unit cells can be found. For simplicity in presentation, we only give specific results for the $\delta$-function case: $V = g_0 d \sum \delta(x - x_n)$, where $g_0$ is the average potential height in a unit cell for the original lattice without field. The rectangular potentials are replaced by $\delta$-functions so that in each unit cell the particle is only scattered once. The unit-cell transfer matrix is shown as follows:

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \begin{pmatrix} 1 + w_n h_n^{(1)}(x_n) / h_n^{(0)} & w_n h_n^{(2)}(x_n) / h_n^{(0)} \\ -w_n h_n^{(3)}(x_n) / h_n^{(0)} & 1 - w_n h_n^{(1)}(x_n) / h_n^{(0)} \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix},$$  \tag{248}

where $w_n = 2ml/h^2 (\xi z_n)^{-1/3} g_0 a$, and all the $h_n$'s are products of Hankel functions of argument $z_n = z(na, \xi, E)$, shown as follows: $h_n^{(0)} = H_n^{(1)}(z_n) H_n^{(2)}(z_n) - H_n^{(1)}(z_n) H_n^{(2)}(z_n)$, $h_n^{(1)} = H_n^{(1)}(z_n) H_n^{(2)}(z_n)$, $h_n^{(2)} = H_n^{(1)}(z_n)^2$, and $h_n^{(3)} = H_n^{(1)}(z_n)^2$. The analytical solutions of Eq. (1) are therefore completely determined:

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = T_N \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = \prod_{n=N}^1 M_n \begin{pmatrix} A_0 \\ B_0 \end{pmatrix},$$  \tag{249}

where $A_0, B_0$ are the initial amplitudes of the wavefunction, $T_N$ is the total transfer matrix between $x_0$ and $x_N$, and $M_n$ is the $n$th transfer matrix in Eq. (248). For a complete analysis, one should also consider the transfer matrices connecting the field-free regions, $x < x_0$ and $x > x_N$, with the region in the field, $x_0 < x < x_w$. The final transfer matrix is denoted as $\mathcal{T}_f$. The transmission coefficient $\mathcal{T}$ is related to the final transfer matrix by

$$\mathcal{T} = |\det(\mathcal{T}_f)/(\mathcal{T}_f)_{22}|^2.$$  \tag{250}

### 4.7.4. Field-induced transmission spectral changes

We are interested in the case when the electronic wavelength is comparable with the superlattice constant. Let $k_0 = 2\pi/a$, and $k_e = \sqrt{2mE}/h$. We want to study the transmission problem for the electrons with energies $E$, such that $k_e/k_0 \sim 0.1$ to 10. For instance, if we take $a = 10$ to 50 Å, and $E = 0.01$ to 1 eV, then we find that $k_e/k_0 \sim 0.1$ to 4. To simplify our numerical results, we first define two dimensionless quantities for eigenenergy and electric field strength. We define the dimensionless energy as $\tilde{E} = E/g_0$, where again, $g_0$ is the average barrier height in a unit cell; so if $\tilde{E} = 1$, it means that the eigenenergy is at the average height of the barrier. We also define a dimensionless electric field as $\tilde{\xi} = e\xi a/g_0$, where $e$ is the electron’s charge, and $a$ is the lattice constant, so that $\tilde{\xi}$ can be seen as the relative potential drop within a cell caused by the electric field. We then can study how the transmission spectrum, as shown in Fig. 25, is changed by the electric field.

As we increase the field strength, we find the second gap (gap II) becomes wider, and shifts to the left (lower value), as can be seen from Fig. 25b and c. The shift of the gap is not a surprise, because a similar result is expected from the semiclassical theory for conductivity. However, when we further increase the field strength, the original band structure collapses and gap II disappears;
Fig. 25. Transmission spectrum changed by the electric field. We plot the transmission coefficient vs. the dimensionless eigenenergy of the electron in the electric field in a 200-unit superlattice with the following strengths: (a) $\delta = 0.0$, (b) $\delta = 1.2 \times 10^{-3}$, (c) $\delta = 0.04$, (d) $\delta = 0.06$, (e) $\delta = 0.08$, and (f) $\delta = 0.12$.

the first transmission band is combined with gap II to form a new low-transmission band (Fig. 25e and f). In the final situation, almost the whole spectrum becomes a transmission band, but with significantly different probability for electrons with different energy. This new band structure cannot be obtained by any weak field approximation, and it is not predicted by any semiclassical calculations.

From the changed spectrum, one can obtain the following conclusions: (1) the first gap, which has been studied extensively in the literature, undergoes moderate shifts in the presence of an
electric field, whereas the second gap is greatly expanded for moderate field strength; (2) an electron with an eigenenergy initially at a transmission (conduction) state may become a gap electron in the field and vice versa; (3) as the field strength is increased, the whole spectrum undergoes a drastic reconstruction, i.e. the first transmission band collapses, and then rises again, and merges with gap II to become a lower transmission band. These changes in transmission spectrum will affect the electronic conductivity, and will result, in some cases, in oscillation between negative and positive differential resistances. We now study the transition processes at the transmission band edges.

Fig. 26 shows how the electric field affects the transmission coefficient of the electron at the left and right gap edges; (a) for $E = 15$, a gap point when there is no electric field, is transformed into a transmission point by the electric field when $\delta > 0.06$; (b) for $E = 12$, a transmission point when there is no field, is transformed into a gap state when $0.02 < \delta < 0.05$, and then returned to a transmission point for larger field strengths. In both cases after escaping from the gap, the transmission coefficient increases smoothly over an interval of about 0.1, and then oscillates as the field is increased.

4.7.5. Summary for the linear effects
We have shown that the transmission spectrum of a superlattice may undergo large changes in an electric field. Such changes will show up in electric conductivity of the superlattice. Similar changes have been observed in other properties of semiconductor superlattices such as the electro-optical effects [190,191] As in our present work, these effects are due to modification of states by the field and the resulting Stark–Wannier localization and intersubband resonance-induced delocalization [192]. We have given explicit results for a superlattice with 200 unit-cells ($N = 200$), but similar results concerning the band shifting and the transitions between the transmission and gap states exist for smaller lattices. However, when $N$ is too small (in our case when $N < 25$), Bragg backscattering from the blocking potentials will not be strong enough to
produce a gap, resulting in a lower transmission band sandwiched between two higher ones in the transmission spectrum. In the presence of an electric field, the edges of the lower transmission band is also shifted and the width is widened. For a stronger field, the distinction between the first two bands will disappear, similar to what is shown in Fig. 25f. Finally, we notice that the localization behavior in a disordered or quasiperiodic infinite system in the presence of an electric field has been studied extensively within the tight-binding model [193–195] and it has been found that localization either decays in real space by a power law or sometimes is totally eliminated by the field. It would be interesting to use the present model to study how disorder in a finite system would affect the transmission property and hence the conductivity of the electrons in the electric field.

4.7.6. Multiple conductance in a nonlinear superlattice

In this section we continue to use the Kronig–Penney model in the presence of an external electric field and to study the nonlinear effects introduced by doped layers in a semiconductor superlattice. In particular, we will try to understand the experimentally observed multistability and discontinuity in the current-voltage characteristics of a doped semiconductor superlattice under an homogeneous electric field. Nonlinearity in our model enters through the self-consistent potential that is used to describe the interaction of the electrons with charges in the doped layers. We show that the process of Wannier–Stark localization is slowed down by the nonlinear effect in the doped layers, and that the shrinking and destruction of minibands in the superlattice by the nonlinearity is responsible for the occurrence of discontinuity and multistability in the transport of electrons.

4.7.7. Multistability in electroconductance

There have been considerable interests in the study of transmissions in a nonlinear medium for both electrons and electromagnetic waves. It has been shown that under certain circumstances nonlinearity can enhance transmission by a self-trapped mechanism and by producing and propagating soliton-like waves in the nonlinear media [141,170]. The dynamics for the transmissions is determined by an interplay of nonlinearity and the periodicity (or the lack of it) of the material. In the ballistic regime of semiconductor nanostructures, electric conductance has been found to be related with transmission probabilities of quantum tunneling by an elementary factor of $2e^2/h$ for each quantum channel that connects the outgoing waves with the incident waves [187,188].

Optical switching and multistability in nonlinear periodic structures have been analyzed extensively and observed in experiments since the work of Winful et al. [95,113,196,197]. Electric field induced Stark ladder effect, Wannier–Stark localization and the electro-optical properties and device applications in the semiconductor superlattices (SL), such as GaAs/AlGaAs, have been studied extensively in recent years [181–186,198]. The quantum wave effect becomes significant in such a system because the wavelengths of electrons in it are in the same order of magnitude as the superlattice constant. Recently, there have been renewed interests in the study of the multistability and discontinuity in the current–voltage ($I–V$) diagram of doped semiconductor superlattices, both theoretically [199,200] and experimentally [201]. It has been shown that the formation of charge domains in a superlattice is the reason for multistability in electroconductance. In this section, we present a theoretical analysis and numerical calculations by using a simple model with techniques of self-consistent potentials, to study the electronic transport in a SL. We demonstrate from
a fundamental quantum mechanical point of view how multistability and switching behaviors occur in a nonlinear discrete system.

### 4.7.8. A model with self-consistent potentials

The wave functions of electrons in a superlattice must obey the Pauli’s principle. For simplicity, we assume a decoupling between the longitudinal and transverse degrees of freedom to make the problem one-dimensional. The nonlinearity arises from the self-consistent potentials [202] produced by the accumulation of charges in the doped layers. The superlattice we consider here consists of square-well/square-barrier semiconductor heterostructures, which is a common model representing the mismatch in the minibands between two component materials of the superlattice. We assume that the doped layers are located in the quantum barriers. Following Ref. [202], in the absence of an external field, we write the self-consistent Schrödinger equation for \( \psi(x,t) \):

\[
\dot{\hbar} \frac{\partial}{\partial t} \psi(x,t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) + \int W(t,t';x,x')|\psi(x',t')|^2 dt'dx' \right] \psi(x,t),
\]

where \( V(x) \) is the periodic potentials. We are interested in the time-independent solutions, \( \psi(x,t) = \psi(x) \exp \{i\omega t\} \). In such a case, the kernel is also assumed to be time-independent, and the integral part in Eq. (251) is proportional to the density of charges in the doped layers. If the size of these regions is much smaller than the spatial variations of \( \psi(x) \), the integral part of Eq. (251) can be replaced by the summation of the average contributions of the localized charges inside the wells:

\[
\sum \tilde{W} |\psi(x_n)|^2 \delta x_n;\quad \text{the average kernel in the well, } \tilde{W}, \text{ is proportional to } e^2 n_e / C, \text{ where } e \text{ is the electron charge, } n_e \text{ is the charge density in the doped layer and } C \text{ is the capacitance of that layer.}
\]

For simplicity, we assume that we have very thin doped layers, and use the \( \delta \)-function type of nonlinear barriers to represent the self-consistent potentials; this is an approximation which makes it much easier to obtain an exact solution for this model. The integral in Eq. (251) is hence replaced by the following summation, \( \sum \tilde{w}|\psi(x)|^2 \delta(x - x_n) \), where \( \tilde{w} \) is proportional to \( \tilde{W} \).

When an external electric field is applied along the growth axis of the superlattice, the most fundamental change that the field makes is the breaking of the translational symmetry. The energy levels of neighboring wells are misaligned, which results in the Wannier–Stark localization owing to the turning-off of the resonant tunneling between consecutive wells, shifted absorption edges [198] and widened gap regions in the transmission spectrum [172]. The time-independent Schrödinger equation for the electron in an external electric field \( \varepsilon \), with energy \( E \), and approaching a sample of \( N \) periodic potential barriers is

\[
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + \left[ \sum_{n=1}^{N} g(|\psi|^2) \delta(x - x_n) - e\varepsilon x \right] \psi(x) = E \psi(x),
\]

where \( g(|\psi|^2) = p(g_0 + g_2|\psi|^2) \), \( p \) is the potential strength; \( g_0 \) and \( g_2 \) are the weight factor \( (pg_2 = \tilde{w}) \), representing the linear and self-consistent nonlinear potentials respectively; \( x_n = na \), where \( a \) is the lattice constant. Eq. (252) is very similar to Eq. (245), except that the barrier’s potential now contains a nonlinear term, the strength of which is proportional to the local probability amplitude. As in Section 4.7.3, we define a characteristic length \( l(\varepsilon) = (\hbar^2 / 2me\varepsilon)^{1/3} \), and a dimensionless parameter \( \lambda(\varepsilon) = (2m\hbar^2 e^2 \varepsilon^2)^{1/3} E \) then, it could be shown that between two consecutive \( \delta \)-function scatters, Eq. (252) can be transformed into a Bessel equation of order \((1/3)\)
[172], and the solutions for propagating waves can be expressed as a combination of Hankel functions of the first and second kinds. The wave functions between \( x_{n-1} \) and \( x_n \) consequently are given as follows:

\[
\psi_n(z) = A_n z^{1/3} H^{(1)}_{1/3}(z) + B_n z^{1/3} H^{(2)}_{1/3}(z),
\]

where \( z(x, \varepsilon) = \frac{2\lambda}{3}(1 + \frac{x}{\lambda(\varepsilon)})^{3/2} \), is the new dimensionless coordinate; \((A_n, B_n)\) are amplitude constants, which will be determined later by boundary conditions; and \( H^{(1,2)}_{1/3}(z) \) are the Hankel functions of the first and second kinds, respectively.

### 4.7.9. Multistability and multi-valued conductance

There is a significant difference in the wave functions of a linear lattice and a nonlinear one. For a linear lattice, \( g \) in Eq. (252) is a constant; the superposition principle holds for the waves in entire lattice. However, the same could not be said about a nonlinear lattice. It is possible that electrons with the same incident wave magnitude \( D_A \), may not necessarily give the same output transmissivity, the transmission coefficient of the sample. We calculate the transmission of electrons in a SL in the presence of an external electric field \( \varepsilon \), and use Landauer’s formula to obtain the corresponding conductance. In Fig. 27, we show the transmission coefficient \( T \) (Fig. 27a) and the electric conductance \( G \) (Fig. 27b) as a function of the field strength \( \varepsilon \), for various values of \( g_2 \). In the linear case \((g_2 = 0)\) and for a moderate electric field, the wave-function of the electrons inside each quantum well is localized (W–S localization) and the transmission is reduced due to the field induced reduction of the resonant tunneling between adjacent wells. As the electric field increases, the electrostatic potential energy of the electrons in each QW is enhanced by the amount of \( \epsilon n/e \); if this value becomes comparable to \( \Delta E_g \), the energy gap between two minibands, enhancement in transmission is expected because of the intersubband resonant tunneling [192]. In the case of many minibands this process of enhanced transmission repeats itself also at higher field values resulting in the oscillatory pattern of the continuous curves in Fig. 27. This oscillatory behavior is a manifestation of the competition between W–S localization and the intersubband resonance-induced delocalization. We note that the delocalization effect is completely absent from a single band model. The effects of W–S localization and the intersubband resonance-induced delocalization can be observed through photon absorption and luminescence [181,182,192].

In the case of weak nonlinearity \((g_2 = 0.05\) in Fig. 27), the oscillatory behavior of transmission coefficient and conductance in the field remains similar to the linear case. However, the left and right sides of each peak becomes asymmetric, which means (a) the W–S localization process is slowed down in the presence of nonlinearity in the doped layers, as shown by the smaller slopes of the increasing curves in Fig. 27; and (b) the widths of the minibands shrink in the presence of moderate nonlinearity, so that the intersubband resonances occur in a narrower range of field values, resulting in the rapid drop after \( T \) or \( G \) reaches a peak value. Finally, drastic changes are observed in the case of strong nonlinearity \((g_2 = 0.25\) in Fig. 27). We notice that W–S localization process is further slowed down in an increasing field, whereas the minibands structure is totally destroyed by the nonlinearity, resulting in abrupt changes in transmission and conductance, including the occurrences of discontinuity and multistability. In Fig. 27, we use \( a = 20\) Å, \( N = 40 \), and \( E = 0.32\) eV (this energy is roughly at the center of the second miniband of the linear model). For the barrier strength, we use \( p = 2.0\) eV Å; \( g_2 = 0.05, \) and \( 0.25, \) respectively, with \( g_0 = 1.0 - g_2. \)
Fig. 27. The effects of nonlinearity is shown from (a) the transmission $T-E$ and (b) the conductance $G-E$ diagrams. For small nonlinear parameter $g_2$, the transmission and conductance curves are tilted and shifted; for large $g_2$, multiple transmissions and conductances become possible. The energy is chosen at a value near a band edge, but multistability is also observed at other energies (not shown). Arrows are used to indicate, as examples, the locations of discontinuity. Other parameters are given in the text. The absolute values are used for the field strengths.

Fig. 27 shows only the multistability in transmissions for the electron with energy $E = 0.32$ eV. In order to understand the whole picture of multistability, we draw a contour plot of multistability on the field-energy parameter plane shown in Fig. 28. It can be seen that up to energy $E = 0.4$ eV, there are three transmission bands separated by gaps of different widths, and the first and second transmission bands consist almost entirely of multistable states. It is very interesting that in the presence of nonlinearity the multistable and mono-stable states in the third transmission band form an oscillatory pattern, which is in agreement with Fig. 27. Detailed studies show that the second and third transmission bands actually comes from a single transmission band in the
corresponding linear case; the splitting is due to the nonlinear forces. Another important thing that we notice is that the first transmission band vanishes when field $\varepsilon > 2.1$ kV/cm. Parameters in Fig. 28 are the same as in Fig. 27.

A second model has been used to study the nonlinear effects in the presence of the field in more detail. In this model the doped layers are placed in the middle of the QWs instead of the barriers. After we obtain the conductance $G$ as in the case of Fig. 27, we use the field strength $\varepsilon$ and sample length $Na$ to obtain the voltage $V = Na\varepsilon$, we then use the Ohm’s law to obtain the current, $I = GV$. The current-field characteristic diagram and possible sweep-up and sweep-down paths for this second model are presented in Fig. 29. We use the following parameters for numerical calculations in Fig. 29: for the barrier potential, $g_0 = 1.0$, $g_2 = 0.0$; and for the doped layers, $g_0 = 0.5$, $g_2 = 0.5$. the rest of the parameters are the same as in Fig. 27. We point out that the behavior depicted in Fig. 27 is in qualitative agreement with the experimental results of Ref. [201].

We now go back to the analytical solution. Considering the continuity of $\psi(x_n)$ and the discontinuity of $d\psi/dx$ at $x = x_n$, solutions of Eq. (252) can be expressed by the following recurrence relations:

\[
A_{n+1} = \left[ 1 + w_n |\psi_n|^2 \right] h_n^{(1)} h_n^{(0)} A_n + w_n \frac{|\psi_n|^2}{h_n^{(0)}} \frac{h_n^{(2)}}{h_n^{(0)}} B_n , \tag{254}
\]

\[
B_{n+1} = \left[ 1 - w_n |\psi_n|^2 \right] h_n^{(1)} h_n^{(0)} B_n - w_n \frac{|\psi_n|^2}{h_n^{(0)}} \frac{h_n^{(3)}}{h_n^{(0)}} A_n , \tag{255}
\]
Fig. 29. The current–field characteristic for the second model. Possible sweep-up and a sweep-down paths are shown as the field is either increased or decreased. The current values (small circles) are obtained by calculating the conductance under different fields. It is easy to draw a hysteresis from this diagram. Parameters are given in the text. The absolute values are used for the field strengths.

where \( w_n = \frac{2n+1}{\pi} (z_n) \^ {1/3} \left| \psi_n(z_n) \right|^2 \); all the \( h_n \)'s are products of Hankel functions of \( z_n \). 

\[
h_n^{(0)} = H_{1/3}^{(2)}(z_n) H_{1/3}^{(1)}(z_n) - H_{1/3}^{(1)}(z_n) H_{1/3}^{(2)}(z_n),
\]

\[
h_n^{(1)} = H_{1/3}^{(1)}(z_n) H_{1/3}^{(2)}(z_n),
\]

\[
h_n^{(2)} = H_{1/3}(z_n)^2,
\]

\[
h_n^{(3)} = H_{1/3}^{(1)}(z_n)^2.
\]

The analytical solutions of Eq. (252) are therefore completely given by Eqs. (253)–(255) if the initial amplitudes \( A_0, B_0 \) are known. However, usually one can only assume that one knows the amplitude of the incident wave, \( A_0 \), but not the reflected one, \( B_0 \); besides that one can also assume that \( B_N = 0 \), since there is no barrier to reflect the waves beyond \( x = Na \). It can be easily shown that the recurrence equations (Eq. (254)) and (Eq. (255)) are reversible for every step. In this case, a self-consistent technique can be used, by numerically finding the appropriate transmitted wave amplitude \( A_N \), such that through the reverse transformations the incident amplitude acquires the desired value, and the solution can be verified by directly applying the equations of the forward transformation.

In order to understand the meaning of the solutions, let us estimate the order of magnitudes of the physical quantities that we have been used, and apply the appropriate asymptotic form to the solutions. Take, for instance, a lattice consisting of \( N = 50 \) cells, with lattice constant \( a = 20 \) Å, \( \delta = 10^4 \) V/cm, and \( E = 0.35 \) eV, then \( l = 72.3 \) Å, and \( \lambda = 483 \). This means that \( z \gg 1 \) is true for all the \( x \)'s; the use of asymptotic form of the Bessel functions is well justified.

\[
H_{1/3}^{(1,2)}(z) \approx \frac{2}{\sqrt{\pi z}} \exp \left\{ \pm i \left( z - \frac{\sqrt{\pi}}{2} - \frac{\pi}{4} \right) \right\},
\]

(256)

where \( v \) is the order of the Hankel function. Eqs. (253)–(255) can be simplified by using Eq. Eq. (256), and the recursion relations can be written as

\[
\tilde{A}_{n+1} = \eta [1 + w_n(\psi_n^2)] \tilde{A}_n + \eta w_n(\psi_n^2) \tilde{B}_n \exp \{ -2ik(x_n) x_n \},
\]

(257)

\[
\tilde{B}_{n+1} = \eta [1 - w_n(\psi_n^2)] \tilde{B}_n - \eta w_n(\psi_n^2) \tilde{A}_n \exp \{ 2ik(x_n) x_n \},
\]

(258)
where $\eta = (z_n/z_{n+1})^{-1/6}$, $\bar{A}_n = \sqrt{(2/\pi)}z_n^{-1/6}A_n \exp(i\theta)$, and $\bar{B}_n = \sqrt{(2/\pi)}z_n^{-1/6}B_n \exp(-i\theta)$, with $
olimits \theta = (2/3)\lambda^{3/2} - (5/12)\pi$. The electron is gaining kinetic energy in the field, and its “wavenumber” $k(x)$ is an increasing function of $x$, given by

$$k(x) = k_0 \left[ 1 + \frac{1}{4} \lambda^{-3/2} k_0 x^2 - \frac{1}{24} \lambda^{-3} k_0^2 x^3 + \ldots \right],$$

where $k_0 = \sqrt{2mE/h}$. The asymptotic solution then can be seen as a modified plane wave.

$$\psi_n(x) = (z_n/z)^{1/6} \bar{A}_n \exp(ik(x)x) + (z_n/z)^{1/6} \bar{B}_n \exp(-ik(x)x). \quad (259)$$

The asymptotic relations are useful in that it helps to illustrate the physical processes, and have been found to be quite reliable for the parameters that we have used. Nevertheless, all the physical quantities of our interests can be calculated directly from Eqs. (253)–(255).

We have demonstrated that the occurrence of multistability and discontinuity in the transport processes of electrons can be explained by introducing the self-consistent potentials to represent the nonlinear space charge effects in the doped semiconductor layers. We use a simple model in which the doped layers are assumed to be ultrathin and provide nonlinear impacts on the wave packages of the electrons. One of the advantages of this model is that a fully quantum-mechanical treatment can be applied without using an effective Hamiltonian. Comparing with the tight-binding model, which is good only for weakly coupled QWs heterostructure, our model inherently creates a series of minibands (multiple conduction subbands structure), and the interwell coupling of the wave functions of all the QWs is fully considered in our algorithm. These couplings are responsible for tunneling and transmission of electrons, and become increasingly important in a superlattice fabricated with thinner barriers. This model can be easily modified to study other heterostructures in an electric field, such as a SL consisting of alternative $n$ and $p$-doped layers and the modulations made by impurity and disorder.

5. Conclusions

We have demonstrated that simple nonlinear lattice systems such as the ones formed through the discrete nonlinear Schrödinger equation and its generalizations can be used to model several physical circumstances ranging from polaron and soliton like problems to nonlinear electrical and optical problems. The main virtue of DNLS-like models is their simplicity, viz. with relatively simple formalism one can describe complicated phenomena. In many cases, such as the one of the nonlinear photonic band gap systems, one can bypass completely the complexity of the real problem while sacrificing only in the quantitative aspects of the results.

In this review we addressed primarily transfer properties of nonlinear lattices. The stationary lattice problem becomes then equivalent to an effective dynamical system described through a nonlinear map whose dynamics corresponds to discrete propagation on the lattice. The map properties are then investigated though the use of standard analytical and numerical techniques. The map associate with the DNLS-AL equation shows rich behavior and different regimes.
depending on the relative strengths of the “integrable” to the “non-integrable” nonlinear terms. We saw that the integrable map regime can be extended to substantial values of the nonlinearity coefficient of the local nonlinear term. The nonintegrable regime is characterized by sensitivity in the initial condition dependence leading, in the lattice problem, to nonpropagating stationary states. The latter do not contribute in the lattice transfer properties.

One interesting application of nonlinear lattices is in one dimensional nonlinear photonic band gap systems. In these systems there is an interplay between nonlinearity and the presence of gaps in the linear band leading to selective amplitude dependent transmission, or switching. We showed some of these properties through a straightforward many band generalization of DNLS, viz. a nonlinear Kronig–Penney model with delta functions. Since in proper variables this system corresponds to a DNLS equation with wavevector dependent nonlinearity coefficient, we used the map approach to study its transmission properties. We also addressed transfer properties in the presence of external fields, targeting semiconductor superlattice applications. We saw that several of the conclusions arrived through the map method can represent qualitatively results obtained experimentally.

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