Chapter 13
Few-Lattice-Site Systems of Discrete Self-Trapping Equations

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13.1 Introduction

In this section, we will review work on few-lattice-site systems of the so-called discrete self-trapping (DST) equations where we will discuss the integrability of few-lattice-site DST systems, the presence of chaos in nonintegrable ones, their applications as well as experimental observations of the systems.

The DST equation which is a generalization of the discrete nonlinear Schrödinger (DNLS) equation was introduced by Eilbeck, Lomdahl, and Scott in [1]. The equation takes the form

$$i\frac{d}{dt}\mathbf{A} + \Gamma\mathbf{D}\left(|\mathbf{A}|^2\right)\mathbf{A} + \epsilon M\mathbf{A} = 0, \tag{13.1}$$

where $\mathbf{A} = \mathrm{col}(\mathbf{A_1}, \mathbf{A_2}, \ldots, \mathbf{A_n})$ is a complex n-component vector and $\mathbf{D}$ is an $n \times n$ matrix denoting the nonlinearity, given by

$$\mathbf{D}\left(|\mathbf{A}|^2\right) \equiv \mathrm{diag}\left(|\mathbf{A_1}|^2, |\mathbf{A_2}|^2, \ldots, |\mathbf{A_n}|^2\right). \tag{13.2}$$

The parameter vector $\Gamma = (\gamma_1, \gamma_2, \ldots, \gamma_n)$ denotes the strength of the nonlinearity. The matrix $M = [m_{jk}]$ is a real symmetric matrix ($m_{jk} = m_{kj}$) representing the linear dispersive interactions between the jth and kth site with the constant strength ϵ. When the $n \times n$ matrix M is taken explicitly as the tridiagonal matrix

$$M = \begin{bmatrix} 0 & 1 & 0 & \ldots & 0 & 1 \\ 1 & 0 & 1 & 0 & \ldots & 0 \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ 0 & \ldots & 0 & 1 & 0 & 1 \\ 1 & 0 & \ldots & 0 & 1 & 0 \end{bmatrix}, \tag{13.3}$$

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the DST equation is then nothing else but the 1D DNLS equation[1] with a periodic boundary condition (see also, e.g., [2] for a brief review of the DNLS over the last two decades). The higher dimensional DNLS equation[2] can also be written in the general form (13.1) with a properly defined matrix M.

The DST equation (13.1) can be derived from the conservation of the Hamiltonian/energy

$$H = -\sum_{j=1}^{n} \left(\frac{\gamma_j}{2} |A_j|^4 + \epsilon \sum_k m_{jk} A_j^* A_k \right) \tag{13.4}$$

with the canonical variables $q_j = A_j$ and $p_j = iA_j^*$. Equation (13.1) also conserves the norm

$$N = \sum_j |A_j|^2. \tag{13.5}$$

Historically, one of the original motivations of the formulation of the DST equation (13.1) was to investigate the self-trapping of vibrational energy in molecular crystals and proteins [1, 3]. The term "self-trapping" itself, which is also called self-localization, refers to an inhibition of the energy dispersion of a coupled nonlinear oscillators system. The concept was introduced long ago in a note by Landau [4] on the motion of a (localized) electron in a crystal lattice.

As one can consider a general choice of matrix M representing longer range couplings or different topologies of the lattice, it is also possible to extend the definition of matrix $\mathbf{D}$. In this case, one will obtain a generalized DST system. As a particular instance, for the same coupling matrix M (13.3), choosing

$$\mathbf{D}(|\mathbf{A}|^2) = \begin{bmatrix} 0 & |A_1|^2 & 0 & \dots & 0 & |A_1|^2 \\ |A_2|^2 & 0 & |A_2|^2 & 0 & \dots & 0 \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ 0 & \dots & 0 & |A_{n-1}|^2 & 0 & |A_{n-1}|^2 \\ |A_n|^2 & 0 & \dots & 0 & |A_n|^2 & 0 \end{bmatrix} \tag{13.6}$$

yields the integrable Ablowitz–Ladik (AL) model on the periodic domain.

Looking at the DST equation (13.1) as a model of the nonlinear dynamics of molecules, including small polyatomic ones such as water, ammonia, methane, acetylene, and benzene [5], it is then suggestive to consider the DST system for small n, i.e., few-lattice-site systems of DST equations. The case of $n = 1, 2, 3,$ and 4 has been originally studied in detail in [1] which describes the molecular

[1] See Chap. 2 of this book.
[2] See Chaps. 3 and 4 of this book.

stretching vibrations in water ($n = 2$), ammonia ($n = 3$), and methane ($n = 4$) [1, 5]. Theoretically, the study of few-lattice-site systems is of interest by itself as is shown later on that the finite size of the system can bring up nontrivial properties, such as an instability to a (stable in the infinite system) coherent structure [6] and a nonstandard type of bifurcation in the study of modulational instabilities of a small size system [7].

13.2 Integrability

When $n = 1$, the DST equation (monomer) becomes an uncoupled nonlinear oscillator

$$i\frac{d}{dt}A_1 + \gamma_1|A_1|^2A_1 = 0,$$

which is integrable and can be solved analytically. It is straightforward to see that the solution is

$$A_1 = 0,\ \pm A_1(0)e^{i\gamma_1 A_1(0)^2 t} \tag{13.7}$$

with the norm $N = 0,\ A_1(0)^2$, respectively.

When $n = 2$ (dimer), the DST

$$\begin{aligned} i\frac{d}{dt}A_1 + \gamma_1|A_1|^2A_1 + \epsilon A_2 &= 0, \\ i\frac{d}{dt}A_2 + \gamma_2|A_2|^2A_2 + \epsilon A_1 &= 0 \end{aligned} \tag{13.8}$$

is also exactly integrable. It is so by the Liouville–Arnold theorem (or Liouville–Mineur–Arnold theorem) [8, 9], since the degree of freedom is equal to the number of conserved quantities, i.e., H (13.4) and N (13.5).

The dimer (13.8) is the simplest few-lattice-site DST system where one can observe the notion of a self-trapping transition, i.e., a transition from a self-trapped state to a non-self-trapped (oscillating) one. To study it, let us consider the system with a uniform nonlinearity strength $\gamma_1 = \gamma_2 = \gamma$, which is scaled to $\gamma = 1$, subject to the completely localized initial condition

$$A_1(0) = 1,\ A_2(0) = 0. \tag{13.9}$$

The dimer (13.8) is then solved numerically for several values of the coupling constant ϵ.

When ϵ is small enough, it is natural to expect that the dynamics of $A_1(t)$ and $A_2(t)$ will resemble the case of the integrable monomer Eq. (13.7). It is indeed the case as is presented in the top left panel of Fig. 13.1 for $\epsilon = 0.1$. By defining the

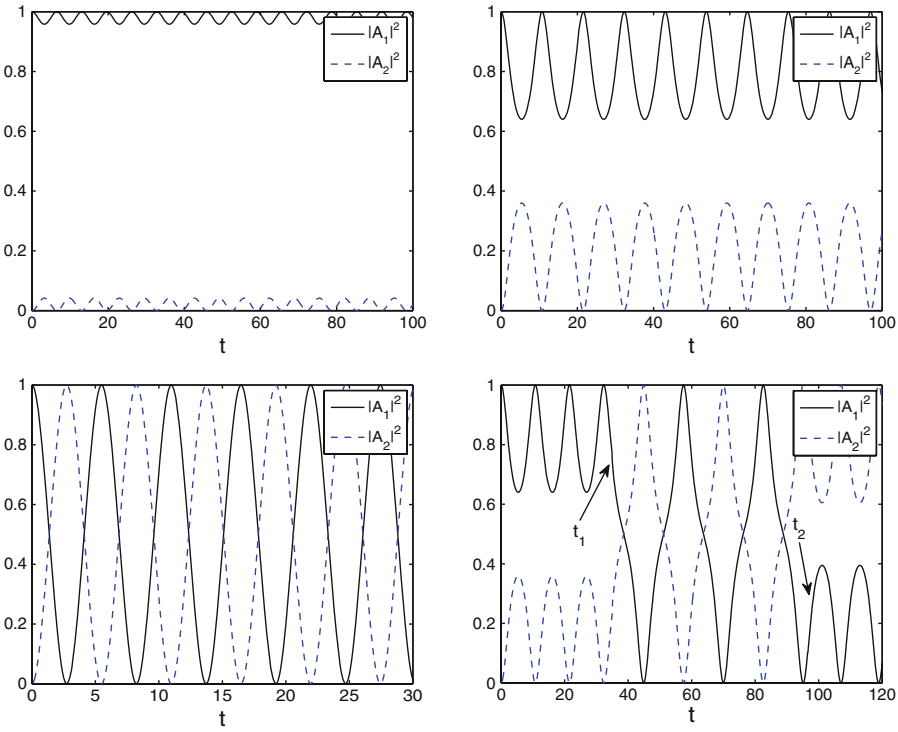

Fig. 13.1 The dynamics of the initial condition (13.9), governed by the DST dimer Eq. (13.8), for several values of the coupling constant ϵ. See the text for the details

so-called site-occupation probability difference $p = |A_1|^2 - |A_2|^2$, it can be seen that even though p is oscillating, it is sign definite. This is the state we refer to as a self-trapped state.

For a slightly larger value of ϵ, e.g., $\epsilon = 0.24$, the dynamics of the initial condition (13.9) still belongs to a self-trapped state, as is plotted in the top right panel of Fig. 13.1. It is clearly indicated that the oscillation period increases as a function of the coupling ϵ.

If ϵ is increased further, there is a critical value of the coupling constant ϵ_{cr} above which the dynamics belongs to a different state. An example is $\epsilon = 0.6 > \epsilon_{\text{cr}}$, depicted in the bottom left panel of Fig. 13.1. It can be deduced that the site-occupation probability difference p is no longer sign definite, which corresponds to a non-self-trapped state and is usually referred to as a Josephson oscillation or a Josephson tunneling state.

Regarding the dynamics of $|A_j|^2$, $j = 1, 2$, Kenkre and Campbell [10] interestingly showed that p satisfies a ϕ^4 equation. This then implies that the general solutions of (13.8) can be written explicitly in terms of the Jacobi elliptic functions. Later, it was also shown [11, 12] that by writing $\dot{q} = \gamma p$, then q will satisfy the sine-Gordon equation. Using the analytical results in [10], the above self-trapping

transition can be clearly observed as one varies ϵ, e.g., that at the critical coupling $\epsilon_{\rm cr}$ the oscillation period becomes infinite.

Later on, Khomeriki et al. [13, 14] demonstrated that the dynamics of $|A_j|^2$ can be controlled through varying the coupling constant for a short time period, such that Josephson oscillations and self-trapped states coexist. The bottom right panel of Fig. 13.1 depicts an example of this. In the panel, the coupling constant is generally set to $\epsilon = 0.24$. Yet, the state can be made to change from initially self-trapping to oscillating by instantaneously setting $\epsilon = 1$ at the point indicated as t_1 for a time period $\Delta t = 0.1$. The Josephson oscillation state has also been made to change to a self-trapped one by setting $\epsilon = 0$ at t_2 for the same period of time.

Besides the DST dimer Eq. (13.8), several generalizations of integrable dimers have been derived and studied as well. An example is the dimer studied by Scott and Christiansen [15]:

$$\begin{aligned} i\frac{d}{dt}A_1 + \gamma|A_1|^{2\sigma}A_1 + \epsilon A_2 = 0, \\ i\frac{d}{dt}A_2 + \gamma|A_2|^{2\sigma}A_2 + \epsilon A_1 = 0, \end{aligned} \tag{13.10}$$

where σ is a non-negative integer. The system is integrable as it conserves the same norm (13.5) and the Hamiltonian

$$H = -\frac{\gamma}{\sigma}[|A_1|^{2+2\sigma} + |A_2|^{2+2\sigma}] - \epsilon(A_1^* A_2 + A_1 A_2^*).$$

Jørgensen et al. [16] showed that when the coupling constant ϵ is allowed to be complex-valued, the dimer

$$\begin{aligned} i\frac{d}{dt}A_1 + \gamma_1|A_1|^2 A_1 + \epsilon A_2 = 0, \\ i\frac{d}{dt}A_2 + \gamma_2|A_2|^2 A_2 \pm \epsilon^* A_1 = 0 \end{aligned} \tag{13.11}$$

is integrable.

Another notable dimer is the one derived by Jørgensen et al. [16]:

$$\begin{aligned} i\frac{d}{dt}A_1 + \gamma|A_1|^2 A_2 + \beta_1|A_2|^2 A_2 + \epsilon_1 A_2 + i\alpha A_1 = 0, \\ i\frac{d}{dt}A_2 + \gamma|A_2|^2 A_1 + \beta_2|A_1|^2 A_1 + \epsilon_2 A_1 - i\alpha A_2 = 0, \end{aligned} \tag{13.12}$$

in which the general system possesses blow-up solutions that can also be written in terms of the Jacobi elliptic functions [16–18].

When $n = 3$ (trimer), the DST is not integrable, as well as the case of $n \geq 4$. Nonetheless, Hennig [19, 20] is able to obtain a generalized integrable trimer using

SU(3) notation, where SU(3) is the group of 3×3 unitary matrices with unit determinant. It is a system of eight real first-order ordinary differential equations.

For a general value of n, one integrable system is the well-known AL equation. The reader is also referred to [21] for another two integrable DSTs formulated in terms of Lie–Poisson algebra derived by Christiansen et al. [21], where one of the models is a Toda lattice-like system.

13.3 Chaos

Since the DST equation is not integrable when $n > 2$, it is then expected that the equation will admit Hamiltonian chaos. It is indeed the case as is demonstrated in the first study [1]. The Lyapunov exponent of the DST trimer was calculated and analyzed numerically in [22] confirming the presence of chaos in the system. Another numerical study on trimers in which the third oscillator is a linear one also shows the presence of chaotic regimes for some well-defined values of the nonlinearity and linear coupling parameters [23]. Calculations using a Melnikov method were also presented by Hennig et al. [24], where they showed analytically the presence of homoclinic chaos in the trimer. The idea was to use the integrable DST dimer as the underlying unperturbed system and to treat the additional oscillator as a small perturbation.

A similar idea as [24] was also used to show the presence of chaotic dynamics in the case of $n = 4$, where now the polymer is assumed to consist of two integrable dimers connected by a perturbative coupling [25]. A numerical computation enabled by the presence of Arnold diffusion was also presented to show the presence of chaos in the general $n = 4$ case [26].

The simplest equations describing two coupled quadratic nonlinear ($\chi^{(2)}$) systems ($n = 2$), each of which consists of a fundamental mode resonantly interacting with its second harmonic forming a four degrees of freedom system, have been studied in [27]. A gradual transition from a self-trapping solution to chaotic dynamics when going away from the near integrable limit $n = 1$ has been discussed as well [27].

Chaos can also be made to exist in an integrable model by perturbing it. Using the SU(2) representation, a study of the analytical structure of a harmonically perturbed nonlinear dimer has been done by Hennig [28]. The study shows that in this case, even though the unperturbed system is integrable, chaos is also observed and proven analytically.

13.4 Applications and Experimental Observations

As was already mentioned that one application of the DST equation was to describe experimental observations of anomalous amide resonances in molecular crystals and proteins, the DST (DNLS) equation also has applications in the study of the

propagation of the complex electromagnetic field envelope in the waveguide arrays [29, 30] and the dynamics of bosons cooled to temperatures very near to absolute zero that are confined in external potentials [31].

In the context of Bose–Einstein physics [31, 32], the DST dimer has been proposed to model the tunneling between two zero-temperature Bose-Einstein condensates (BECs) confined in a double-well magnetic trap [33]. Using the so-called Wannier function-based expansion [34], the infinite-dimensional double-well potential problem [35] can be asymptotically reduced to the DST dimer [33, 36]. All the dynamics of the integrable system which have been solved analytically by Kenkre and Campbell [10] find their new interpretation in this context, including the so-called "macroscopic quantum self-trapping" [33, 36] which is nothing else but the self-trapped states observed in [1]. Following the theoretical prediction, successful experiments have been performed confirming the presence of periodic oscillations and self-trapping in the system [37, 38].

Buonsante et al. [39] have also considered trimers where chaotic solutions of the systems are now studied in the context of BECs and argued that they may correspond to macroscopic effects that can be viable to experiments. Pando and Doedel [40, 41] extended the study of few-site DST systems modeling BECs to the case of $n = 3, 5, 7$ with periodic boundary conditions in the presence of a single on-site defect. In the case of the trimer, it is found that $1/f$ noise is a robust phenomenon taking place as a result of intermittency [41]. In the case of $n = 5$ and 7, another robust effect, where chaotic synchronization of symbolic information arises in the Hamiltonian system, is then observed [40]. Related to this multisite DST system, successful experiments on BECs trapped by an optical lattice, that using again Wannier function expansion can be modeled by such DST equations, have been conducted and reported in the seminal paper [42].

In the context of waveguide arrays [29], the study of the DST dimer has actually been done a couple of years before the work [1] by Jensen in his seminal paper [43]. The dimer is used to model the coherent interaction of two optical waveguides placed in close proximity. Jensen also observed the exchange of power between the waveguides which is nothing else but the periodic solutions of Kenkre and Campbell [10]. An experimental observation has been reported as well in this context in which it is shown that in a double-trap potential system, there is a spontaneous symmetry breaking [44], i.e., the ground state of the system becomes asymmetric beyond a critical power N (cf. Eq. (13.5)).

A numerical study on a DST trimer to model a three-waveguide nonlinear directional coupler also has been conducted by Finlayson and Stegeman [45]. In the paper, they reported that transitions from quasi-periodic to chaotic behavior and back take place as the power N is varied.

A similar trimer as the one studied by [24] has been considered as well in the context of an optical coupler configuration consisting of two nonlinear waveguides coupled to a linear one [46, 47]. In relation to its physical context, it is shown that this type of coupler system can act as an optical switching device with switching properties superior to that of conventional two and three all nonlinear coupler configurations.

Experimental observations for the case of systems with a three-well potential have been performed in strontium barium niobate crystals [48]. Corroborated by an analytical study using the Lyapunov–Schmidt reduction method, it is shown that the presence of a third well causes all bifurcations of static solutions to be of saddle node type [48].

Recently, a few-lattice-site $n = 5$ DST system modeling waveguide arrays, i.e., a nonlinear trimer equation coupled to linear waveguides at the boundaries, was also studied by Khomeriki and Leon [49]. They showed that by controlling the intensity of light along the linear waveguides, the middle one can be sensitive to perturbations. The observation then demonstrates that such a system can be utilized as a weak signal detector [49].

13.5 Conclusions

To conclude, we have briefly reviewed the study of few-lattice-site systems of DST equations. It has to be admitted that the present review is far from covering and summarizing all the work that has been done on the subject. As an example, the study of quantum versions of DST equations [3] is totally omitted in this section. Nonetheless, it is expected that this review will give an idea that even in rather simple small-size systems, a lot of interesting problems and nontrivial properties can be observed and possibly technologically exploited. This then indicates that it is of interest to further study few-lattice-site systems of DST equations. One possible direction would be understanding further connections between few-site and many-site systems. As recently showed numerically by Buonsante et al. [7], even investigating the ground states of the system already reveals interesting behaviors, such as coexistence of a single-pulse and a uniform solution in a finite range of the coupling constant when $n < 6$ and the disappearance of the single-pulse mode beyond a critical parametric threshold.

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