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Self-trapping and blow-up in integrable dimers

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Abstract. The Poisson structure and exact solvability of several nonlinear dimers is demonstrated and used to investigate self-trapping and blow-up effects. A large class of nonlinear dimers is shown to be solvable in terms of Jacobi elliptic functions using the r-matrix method.

1. Introduction

In this paper we investigate two nonlinear effects—self-trapping and blow-up—in several modified self-trapping dimers. For these discrete integrable systems we obtain the Poisson structure and demonstrate the exact solvability in four cases with compact and non-compact algebraic structures.

Self-trapping is the phenomenon where the system is confined to only a part of phase space. The simplest example is that of the motion in a double well. Blow-up describes the situation where the solution ceases to exist after a finite time. In physical systems the blow-up will at some stage be countered by dissipative effects.

The discrete self-trapping (DST) system is a set of coupled nonlinear (complex) oscillators, which was introduced by Eilbeck *et al* [1] as a model to describe the nonlinear dynamics of small polyatomic chains such as water, ammonia, methane, acetylene, and benzene, as well as of larger molecules, such as acetanilide. The DST system arises in other fields too, e.g. quasiparticle motion on a dimer [2], stabilization of high-frequency vibrations in the field of acoustic phonons in the Davydov model [3], and in nonlinear optics to describe arrays of coupled nonlinear waveguides [4, 5].

First we discuss a generalization of the DST dimer with two different algebraic structures: compact and non-compact. The terms compact and non-compact refer to the topology of the phase space, i.e. whether the phase space is bounded or not. For compact algebras the motion is always bounded, thus excluding the possibility of blow-up. Non-compact algebras, on the other hand, may exhibit blow-up depending upon the nature of the system. The existence of blow-up is therefore closely related to the underlying algebraic structure. In the compact case we explicitly show the transition from free to self-trapped motion, whereas in the non-compact case we investigate the presence of blow-up.

Then we use the r-matrix method [6] to obtain a generic class of integrable dimers. This method has proven to be applicable to a large number of discrete systems including the Heisenberg spin chain [6], and in this paper we present yet another application. The generic class of dimers thus obtained includes, as special cases, the generalized DST dimer examined above and the near-Toda dimer [7], the latter being a generalization of the Toda lattice that also exhibits blow-up.

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2. The compact case

We first consider the Hamiltonian [8–10]

$$H = \frac{\gamma_1}{2}|A_1|^4 + \frac{\gamma_2}{2}|A_2|^4 + \alpha|A_1|^2|A_2|^2 + \omega_1|A_1|^2 + \omega_2|A_2|^2 + \epsilon A_1^* A_2 + \epsilon^* A_1 A_2^* \qquad (2.1)$$

where the complex site amplitudes A_1 and A_2 satisfy the Poisson structure $\{A_j, A_j^*\} = -\mathrm{i}$, while γ_1, γ_2, α, ω_1, and ω_2 are real parameters and ϵ is complex. ω_1 and ω_2 are onsite eigenfrequencies, γ_1 and γ_2 are onsite nonlinearities, ϵ is a linear coupling parameter, whereas α determines the nonlinear coupling.

The symmetric resonant case with linear coupling, $\gamma_1 = \gamma_2$, $\omega_1 = \omega_2$, and $\alpha = 0$, is solved in [1] and exhibits a phase transition from 'free' to 'self-trapped' behaviour depending on whether the ratio $\tilde{H}/(|\epsilon|N)$ is less than or greater than unity, respectively. Here $\tilde{H}$ is the equivalent Hamiltonian given by (2.4) and N is the 'number' given by (2.2*a*). The quantum-mechanical aspects of the non-resonant case, $\omega_1 \neq \omega_2$, were considered in [11].

Below we shall examine the general case and present a precise definition of self-trapping. In terms of the Feynman variables

$$N = |A_1|^2 + |A_2|^2 \qquad (2.2a)$$

$$r_1 = A_1 A_2^* + A_1^* A_2 \qquad (2.2b)$$

$$r_2 = \mathrm{i}(A_1 A_2^* - A_1^* A_2) \qquad (2.2c)$$

$$r_3 = |A_1|^2 - |A_2|^2 \qquad (2.2d)$$

which satisfy the compact su(2) algebra

$$\{r_1, r_2\} = 2r_3 \qquad (2.3a)$$

$$\{r_2, r_3\} = 2r_1 \qquad (2.3b)$$

$$\{r_3, r_1\} = 2r_2 \qquad (2.3c)$$

$$\{N, r_j\} = 0 \qquad j = 1, 2, 3 \qquad (2.3d)$$

$$N^2 = r_1^2 + r_2^2 + r_3^2 \qquad (2.3e)$$

the Hamiltonian may be written as

$$\tilde{H} = \frac{\gamma}{4}(r_3 + \delta)^2 + \mathrm{Re}\,\epsilon r_1 - \mathrm{Im}\,\epsilon r_2 \qquad (2.4)$$

where $\gamma = (\gamma_1 + \gamma_2 - 2\alpha)/2$, $\delta = [N(\gamma_1 - \gamma_2) + 2(\omega_1 - \omega_2)]/(\gamma_1 + \gamma_2 - 2\alpha)$, and constant terms involving N and N^2 have been omitted. The 'number' N is a Casimir element of the su(2) algebra (2.3*a*–*e*) and is therefore a second conserved quantity, rendering the system completely integrable.

The equations of motion are obtained in the usual fashion via $\dot{F} = \{F, H\}$, which after the canonical transformation

$$\tilde{r}_1 = r_1 \cos\theta - r_2 \sin\theta$$

$$\tilde{r}_2 = r_1 \sin\theta + r_2 \cos\theta$$

with $\epsilon = |\epsilon|\mathrm{e}^{\mathrm{i}\theta}$ become

$$\dot{\tilde{r}}_1 = -\gamma(r_3 + \delta)\tilde{r}_2$$

$$\dot{\tilde{r}}_2 = \gamma(r_3 + \delta)\tilde{r}_1 - 2|\epsilon|r_3$$

$$\dot{r}_3 = 2|\epsilon|\tilde{r}_2.$$

$\tilde{r}_1$ and $\tilde{r}_2$ may also be expressed in terms of r_3 and the conjugate momentum p_3 (in contrast to the conjecture in [12]).

We may get a single first-order ODE for r_3 by the following calculation

$$(\dot{r}_3)^2 = 4|\epsilon|^2(N^2 - \tilde{r}_1^2 - r_3^2)$$
$$= 4|\epsilon|^2(N^2 - r_3^2) - 4\left(\tilde{H} - \frac{\gamma}{4}(r_3+\delta)^2\right)^2. \qquad (2.5)$$

The right-hand side is a fourth-degree polynomial in r_3, and hence $r_3(t)$ may be expressed in terms of Jacobi elliptic functions [13]. Since $r_3^2 \leqslant N^2$ it follows that $r_3(t)$ is bounded at all times, and hence there can be no blow-up in this system. For $\delta = 0$, equation (2.5) can be reduced to a pendulum equation for the variable τ, defined by $\dot{\tau} = r_3$ [14].

In the following we shall investigate the phenomenon of self-trapping for the ODE (2.5). In normalized variables $x = r_3/N$, $\tilde{\delta} = \delta/N$, $K_1 = \tilde{H}/(|\epsilon|N)$, and $K_2 = \gamma N/(4|\epsilon|)$ we obtain

$$\left(\frac{\dot{x}}{2|\epsilon|}\right)^2 = 1 - x^2 - (K_1 - K_2(x+\tilde{\delta})^2)^2. \qquad (2.6)$$

We define self-trapping as the presence of a gap in the positive support of the right-hand side of (2.6). For $\tilde{\delta} = 0$ we thus recover the condition $K_1^2 > 1$ for the existence of self-trapping.

To analyse the general case it is necessary to investigate the location of the zeros of the right-hand side of (2.6). We first note that we may choose $\tilde{\delta} \geqslant 0$ as well as $K_2 \geqslant 0$ without loss of generality by changing the signs of x and K_1, respectively.

The transition from free to self-trapped behaviour is characterized by a double root in the right-hand side of (2.6). Using MATHEMATICA [15] this amounts to the condition

$$c_4K_1^4 + c_3K_1^3 + c_2K_1^2 + c_1K_1 + c_0 = 0 \qquad (2.7)$$

with

$$c_0 = 1 + (8 + 20\tilde{\delta}^2 - \tilde{\delta}^4)K_2^2 + 16(1-\tilde{\delta}^2)^3K_2^4$$
$$c_1 = 2(-4 + \tilde{\delta}^2)K_2 + 8(-1+\tilde{\delta}^2)(4+5\tilde{\delta}^2)K_2^3$$
$$c_2 = -1 + 8(1-4\tilde{\delta}^2)K_2^2 - 16(-1+\tilde{\delta}^2)^2K_2^4$$
$$c_3 = 8K_2 + 32(1+\tilde{\delta}^2)K_2^3$$
$$c_4 = -16K_2^2$$

which is a fourth-degree polynomial giving K_1 as function of K_2 and $\tilde{\delta}$.

When $K_2 < \frac{1}{2}$ there are only two real roots to this equation. For the case $K_2 = 0.2$ they are shown in figure 1(a) as a function of $\tilde{\delta}$. The two roots separate the free region from the void region, the latter corresponding to invalid initial conditions with $(\dot{x})^2 < 0$.

When $K_2 > \frac{1}{2}$ and $\tilde{\delta} < \tilde{\delta}^{\mathrm{cr}}$ there are four roots separating the free and void regions from a region containing self-trapping. When $K_2 > \frac{1}{2}$ and $\tilde{\delta} > \tilde{\delta}^{\mathrm{cr}}$ there are again only two real roots and all the valid initial conditions lead to free behaviour. This is shown in figure 1(b) for the case $K_2 = 2$.

For fixed value of $K_2 > \frac{1}{2}$, equation (2.7) thus determines a window $K_1^-(\tilde{\delta}) < K_1 < K_1^+(\tilde{\delta})$ as function of $\tilde{\delta}$ where the system exhibits self-trapping. When $\tilde{\delta}$ increases beyond $\tilde{\delta}^{\mathrm{cr}}$ this window disappears.

The critical value $\tilde{\delta}^{\mathrm{cr}}$ is determined by requiring (2.7) to have a double root as function of K_1. Thus we are led to the following equation

$$0 = (1-4K_2^2)^3 + 12\tilde{\delta}^2K_2^2(1+28K_2^2+16K_2^4) + 48\tilde{\delta}^4K_2^4(1-4K_2^2) + 64\tilde{\delta}^6K_2^6$$

which has the solution

$$\tilde{\delta}^{\mathrm{cr}} = (1-(2K_2)^{-1/3})^{3/2}. \qquad (2.8)$$

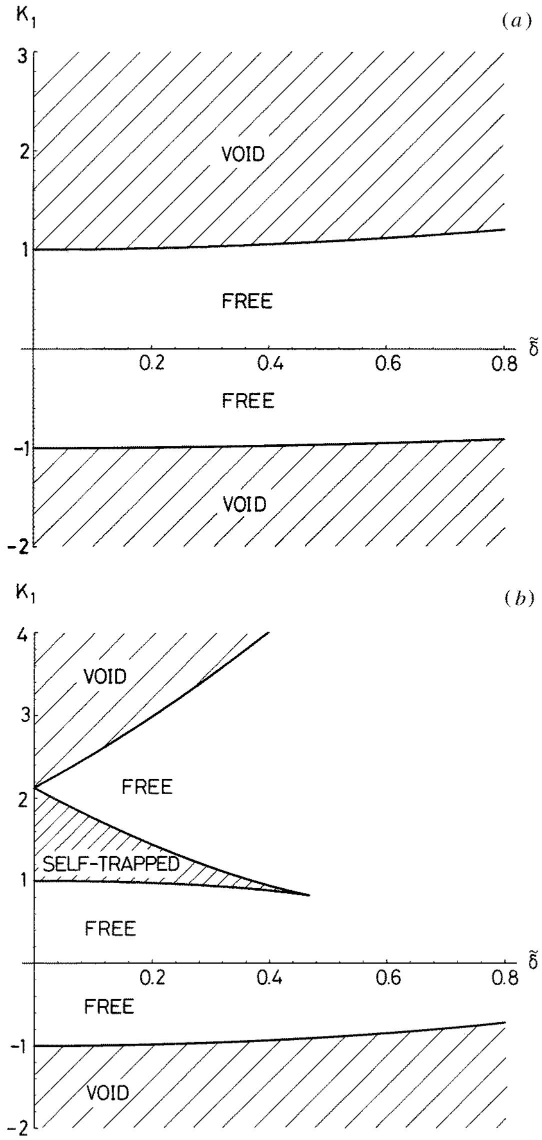

Figure 1. Compact case, phase diagram for $K_2 = (a)$ 0.2, (b) 2.

This critical value tends to the limit 1 as K_2 goes to infinity, and from the definition of $\tilde{\delta}$ we may conclude that for all non-zero values of the parameters γ, δ, and $|\epsilon|$ there exist initial conditions leading to self-trapping. For $K_2 < \frac{1}{2}$ there is no critical value, and all such initial conditions lead to free behaviour.

3. The non-compact case

We now consider the same Hamiltonian (2.1) where the variables this time satisfy the alternate Poisson brackets $\{A_1, A_2^*\} = \{A_2, A_1^*\} = -\mathrm{i}$. The Feynman variables (2.2*a*–*d*) now satisfy the non-compact su(1, 1) algebra

$$\{r_2, r_3\} = -2N \tag{3.1a}$$

$$\{r_3, N\} = 2r_2 \tag{3.1b}$$

$$\{N, r_2\} = 2r_3 \tag{3.1c}$$

$$\{r_1, N\} = \{r_1, r_2\} = \{r_1, r_3\} = 0. \tag{3.1d}$$

The Casimir element r_1 satisfies $r_1^2 = N^2 - r_2^2 - r_3^2$ and is a second conserved quantity, rendering the system completely integrable. The Hamiltonian may be written as

$$\tilde{H} = r_2^2 \frac{\gamma_1 + \gamma_2 + 2\alpha}{8} + r_3^2 \frac{\gamma_1 + \gamma_2}{4} + N r_3 \frac{\gamma_1 - \gamma_2}{4} + N \frac{\omega_1 + \omega_2}{2} + r_3 \frac{\omega_1 - \omega_2}{2} - r_2 \mathrm{Im}\,\epsilon \tag{3.2}$$

omitting constant terms involving r_1 and r_1^2. Because the algebra is non-compact it raises the possibility of blow-up. As shown in [8] this indeed happens for certain parameter values, in particular when $\gamma_1 = \gamma_2 \equiv \gamma$, $\omega_1 = \omega_2 = \epsilon = 0$, with $\alpha > -\gamma > 0$.

In the following we shall investigate the symmetric case $\gamma_1 = \gamma_2 \equiv \gamma$ and $\omega_1 = \omega_2 \equiv \omega$, with the corresponding Hamiltonian

$$\tilde{H} = r_2^2 \frac{\gamma + \alpha}{4} + r_3^2 \frac{\gamma}{2} + N\omega - r_2 \mathrm{Im}\,\epsilon. \tag{3.3}$$

This system may be reduced to a generalized pendulum equation as shown below.

We introduce the time variable τ via $\dot{\tau} = r_3$. The equations of motion become

$$\frac{\mathrm{d}N}{\mathrm{d}\tau} = (\alpha - \gamma)\left(r_2 + \frac{2\mathrm{Im}\,\epsilon}{\alpha - \gamma}\right)$$

$$\frac{\mathrm{d}r_2}{\mathrm{d}\tau} = -2\gamma\left(N + \frac{\omega}{\gamma}\right)$$

which have the solution

$$N = \frac{\Omega A}{2\gamma} \sin \Omega\tau - \frac{\omega}{\gamma} \tag{3.4a}$$

$$r_2 = A \cos \Omega\tau - \frac{2\mathrm{Im}\,\omega}{\alpha - \gamma} \tag{3.4b}$$

where $\Omega^2 = 2\gamma(\alpha - \gamma)$ and $A^2 = 4\tilde{H}/(\alpha - \gamma)$ plus constant terms. The equation of motion for r_3 then leads to the generalized pendulum equation

$$\ddot{\tau} = A^2 \Omega \frac{\alpha + \gamma}{4\gamma} \sin 2\Omega\tau - \omega A \frac{\alpha - \gamma}{\gamma} \cos \Omega\tau - \frac{4A\mathrm{Im}\,\epsilon\gamma}{\Omega} \sin \Omega\tau. \tag{3.5}$$

Like the pendulum equation, the solution to this equation may be expressed in terms of Jacobi elliptic functions.

We now investigate the appearance of blow-up for the ODE (3.5). For $\alpha/\gamma < 1$ we find that Ω becomes imaginary. Inserting $\Omega = \mathrm{i}\sigma$, $\sigma > 0$, into (3.5) and keeping only the first term on the right-hand side leads to

$$\ddot{\tau} \approx -\frac{A^2\sigma}{4}\left(\frac{\alpha}{\gamma} + 1\right) \sinh 2\sigma\tau.$$

Since from (3.4*a*–*b*) it follows that A is real, we see that the system blows up when $\alpha/\gamma + 1 < 0$.

In the next section we will show how to integrate this system in terms of Jacobi elliptic functions.

4. A general integrable dimer

In the following we will derive a generic class of Hamiltonians solvable by the r-matrix method. Then we will show that this class includes the previous dimers as special cases.

Define the 2×2 transfer matrices [16]

$$L_j(u) = \begin{pmatrix} b_j(u + \kappa p_j q_j) - a_j & \kappa \rho_j p_j \\ q_j & d_j(u - \kappa p_j q_j) + c_j \end{pmatrix} \qquad j = 1, 2 \tag{4.1}$$

with $\rho_j = b_j c_j + a_j d_j - \kappa b_j d_j p_j q_j$, $\{q_j, p_k\} = \delta_{jk}$, and a_j, b_j, c_j, d_j, and κ arbitrary constants. u is the spectral parameter. The transfer matrices $L_j(u)$ satisfy the Poisson algebra [6]

$$\{L(u) \overset{\otimes}{,} L(v)\} = [r(u - v), L(u) \otimes L(v)] \tag{4.2}$$

where $\otimes$ denotes the usual tensor product, $[A, B]$ denotes the commutator of the matrices A and B, and $\{\cdot \overset{\otimes}{,} \cdot\}$ is the tensor product with element multiplication replaced by the Poisson bracket. The matrix $r(u)$ is given by

$$r(u) = \frac{\kappa}{u} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{4.3}$$

It can been shown [6] that the monodromy matrix $L(u) = L_1(u) \cdot L_2(u)$ satisfies (4.2) too, and that its trace

$$t(u) \equiv \mathrm{tr}(L_1(u) \cdot L_2(u))$$

is a generating function for integrals of motion in involution.

For the choice (4.1) we obtain

$$t(u) = (b_1 b_2 + d_1 d_2)u^2 + \mathcal{J}_1 u + \mathcal{J}_2 \tag{4.4}$$

where the commuting variables $\mathcal{J}_1$ and $\mathcal{J}_2$ are functions of p_1, p_2, q_1, and q_2. They may conveniently be written in terms of Feynman variables now defined by

$$N = p_1 q_2 - p_2 q_1 \tag{4.5a}$$

$$r_1 = p_1 q_1 + p_2 q_2 \tag{4.5b}$$

$$r_2 = p_1 q_2 + p_2 q_1 \tag{4.5c}$$

$$r_3 = p_1 q_1 - p_2 q_2 \tag{4.5d}$$

which satisfy the su(1, 1) algebra (3.1*a*–*d*) given in section 3. Thus the Casimir element r_1 is a second conserved quantity. We then obtain

$$\mathcal{J}_1 = \kappa(b_1 b_2 - d_1 d_2) r_1 + c_1 d_2 + c_2 d_1 - a_1 b_2 - a_2 b_1$$

$$\mathcal{J}_2 = \kappa H + g_0 + g_1 r_1 + g_2 r_1^2$$

for some constants g_0, g_1, and g_2. The Hamiltonian H assumes the form

$$H = k_1 N + k_2 r_2 + k_3 r_3 + k_4 N r_3 + k_5 r_2 r_3 + k_6 r_3^2 \tag{4.6}$$

where

$$k_{1,2} = \frac{1}{2}(b_1 c_1 \mp b_2 c_2 + a_1 d_1 \mp a_2 d_2) - \frac{\kappa r_1}{4}(b_1 d_1 \mp b_2 d_2)$$

$$k_3 = \tfrac{1}{2}(a_1 b_2 - a_2 b_1 + c_1 d_2 - c_2 d_1)$$

$$k_{4,5} = -\frac{\kappa}{4}(b_1 d_1 \pm b_2 d_2)$$

$$k_6 = -\frac{\kappa}{4}(b_1 b_2 + d_1 d_2).$$

It follows from the above that any Hamiltonian of the form (4.6) is completely integrable. We will now show how the r-matrix method may be used to integrate the Hamiltonian (4.6) in terms of Jacobi elliptic functions.

The powerful method of separation of variables has been shown to be applicable to systems represented by a monodromy matrix satisfying (4.2) with the r-matrix (4.3), see for instance the recent review [17]. Let u_j be the roots of the lower left-hand element of the monodromy matrix $L(u)$. These variables then satisfy the so-called Dubrovin equations [18]

$$\dot{u}_j = \sqrt{R(u_j)} \prod_{k \neq j} \frac{1}{u_j - u_k}$$

with $R(u) = t(u)^2 - 4 \det L(u)$, where $t(u)$ is given in (4.4). For the choice (4.1) we have the single separation variable u_1 given by

$$u_1 = \frac{q_2(\kappa d_1 p_1 q_1 - c_1) - q_1(\kappa b_2 p_2 q_2 - a_2)}{d_1 q_2 + b_2 q_1}$$

and it therefore satisfies

$$(\dot{u}_1)^2 = ((b_1 b_2 + d_1 d_2) u_1^2 + \mathcal{J}_1 u_1 + \mathcal{J}_2)^2 \\ -4(b_1 u_1 - a_1)(d_1 u_1 + c_1)(b_2 u_1 - a_2)(d_2 u_1 + c_2). \qquad (4.7)$$

The right-hand side of (4.7) is of fourth degree in u_1 and the solution $u_1(t)$ may therefore be expressed in terms of Jacobi elliptic functions. It can be shown that the shifted and scaled variable $\tilde{u}_1 = (u_1 - a_2/b_2)/\kappa$ may be expressed in terms of the parameters $k_1, \ldots, k_6$ and the variables N, r_1, r_2, and r_3. We have thus given the solution for an arbitrary Hamiltonian of the form (4.6).

We now show that the general system (4.6) reduces to the non-compact case for special choices of the parameter values. Introducing the canonical transformation

$$\tilde{r}_2 = r_2 \cos\theta - r_3 \sin\theta$$
$$\tilde{r}_3 = r_2 \sin\theta + r_3 \cos\theta$$

and choosing the parameter θ such that

$$\cos^2\theta = -\frac{\gamma}{\alpha}$$

gives the equivalent Hamiltonian

$$\bar{H} = \left(\gamma + \frac{\alpha}{2}\right) \tilde{r}_3^2 + \sqrt{-\gamma(\alpha+\gamma)}\,\tilde{r}_2 \tilde{r}_3 - \operatorname{Im}\epsilon \sqrt{\frac{\alpha+\gamma}{\alpha}}\,\tilde{r}_2 + \operatorname{Im}\epsilon \sqrt{-\frac{\gamma}{\alpha}}\,\tilde{r}_3 + \omega \tilde{N}$$

which is of the form (4.6).

Another special case of the general Hamiltonian (4.6) is obtained by setting $b_1 = b_2 = 1$, $c_1 = c_2 = c$, $d_1 = d_2 = 0$, and $\kappa = -1/m$. Applying the canonical transformation $Q_j = \log q_j$ and $P_j = p_j q_j$, $j = 1, 2$, then leads to the Hamiltonian

$$H = \frac{m}{2}\left(\frac{P_1}{m} + a_1\right)^2 + \frac{m}{2}\left(\frac{P_2}{m} + a_2\right)^2 + c(P_1 \exp(Q_2 - Q_1) + P_2 \exp(Q_1 - Q_2)) \qquad (4.8)$$

omitting constant terms. This is the near-Toda lattice specialized to two degrees of freedom. It was first introduced in [7] as an integrable generalization of the Toda lattice [19].

5. Conclusions

We have presented a detailed analysis of two dimers and demonstrated the presence of self-trapping and blow-up. In particular we found for the Hamiltonian (2.4) the following conditions for self-trapping:

(i) $K_2 > \frac{1}{2}$,

(ii) $\tilde{\delta} < \tilde{\delta}^{\mathrm{cr}}$,

(iii) the left-hand side of (2.7) must be negative, and

(iv) the right-hand side of (2.6) must be positive.

For the Hamiltonian (3.3) we showed that blow-up is present provided $\alpha/\gamma + 1 < 0$.

Finally we showed that the general Hamiltonian (4.6) may be integrated in terms of Jacobi elliptic functions and that it contains two interesting special cases: the generalized DST dimer (3.3) and the near-Toda dimer (4.8).

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