MEL'NIKOV ANALYSIS OF PHASE SPACE TRANSPORT IN A N–DEGREE–OF–FREEDOM HAMILTONIAN SYSTEMS

VASSILIOS M. ROTHOS1, TASSOS C. BOUNTIS1 1Department of Mathematics, University of Patras, GR-261.10 Patras, Greece.
rothos—bountis@math.upatras.gr

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1. INTRODUCTION

The existence of homoclinic (or heteroclinic) orbits, i.e trajectories connecting saddle fixed points of systems of differential equations (odes) is of special significance in virtually all applications in which such solutions arise. For example, homoclinic orbits have been shown to underlie certain phenomena of intermitency in fluid mechanics [6]. There are also examples where homoclinic orbits play an important role in the chaotic behavior of electrical circuits [8]. In nonlinear optics it has been shown that homoclinic orbits can be responsible for the chaotic behavior of lasers as well as light pulses in fiber optics applications [7], or the chaotic behavior arising in structural mechanics [9].

Unfortunately, there are few analytical methods for proving the existence (or nonexistence) of homoclinic orbits, in a given system of odes. For 2D problems, saddle connections can be studied by standard phase plane techniques. However, the situation becomes especially difficult for systems whose phase space is of dimension larger than two. The most widely applicable approach in this direction is the so–called *Mel'nikov method* [1], which is global perturbation method, utilizing the geometrical features of integrable Hamiltonian systems as a framework in which to develop analysis. The unperturbed system is an integrable Hamiltonian system having a normally hyperbolic invariant set whose stable and unstable manifolds intersect nontransversely [13]. The global geometry associated with the integrable structure serves to develop coordinates which are used to determine if any of the homoclinic orbits in the normally hyperbolic invariant set survives under perturbation.

In this paper, we consider the discrete nonlinear Schrodinger equation (DNLS)

$$i\,\dot{c}_j = -\gamma |c_j|^2 c_j - \left(W_{j,j+1} c_{j+1} + W_{j,j-1} c_{j-1}\right) \quad j = 1, \cdots, n \tag{1.1}$$

where c_j is a complex probability amplitude at site j, γ is the local nonlinearity parameter and $W_{j,j\pm1}$ are the dispersion parameters determining the linear coupling between the sites.

The Discrete Nonlinear Schrodinger Equation (DNLS) or Discrete Self-Trapping Equation (DST) [4] 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 the enviroment 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 understand nonlinear localization phenomena. It can also be viewed as an equation describing the motion of a quantum mechanical particle interacting strongly with vibrations. Typically, an infinite, discrete set of equations is viewed in two different ways: either as a discretization of a corresponding continuous field equation, or an equation describing dynamics in discrete lattices. In the DNLS case, the corresponding continuous field equation is the celebrated Nonlinear Schrodinger Equation. Here, however, we will take the point of view that (1.1) represents the dynamics in a discrete, 1–dimensional lattice.

We study the intgrability of the 5–element DNLS pentamer, as an example of the general N–dimensional case. We prove the existence of chaotic solutions analytically. Starting from an integrable dimer and treating the weak coupling to the remaining sites of the 5-mer configuration perturbationally, we prove the existence of homoclinic tangles by applying Mel'nikov 's method following Wiggins [13] and study the appearence of diffusion and transport in phase space in the coupled oscillator system [12].

2. THE DNLS PENTAMER AND SYMMETRY REDUCTION

We write the DNLS pentamer Hamiltonian in terms of the complex site occupation amplitudes as:

$$H = H_0 - \epsilon[\sum_{k=2}^{5} W_{1k}(c_k^* c_1 + c_1^* c_k) + \sum_{k=3}^{5} W_{2k}(c_k^* c_2 + c_2^* c_k) + \sum_{k=4}^{5} W_{3k}(c_k^* c_3 + c_3^* c_k)] \tag{2.1a}$$

$$H_0 = -\frac{1}{2}\gamma \sum_{j=1}^{5} |c_j|^4 - W_{45}(c_4^* c_5 + c_5^* c_4) \tag{2.1b}$$

The system is assumed to be symmetric in the nonlinearity parameters $\gamma_j = \gamma$ as well as in the on–site energies $E_j = E$ $(j = 1, \cdots, 5)$, while for the dispersion parameters, $W_{ij} = W_{ji}$, we have chosen much stronger coupling $W_{45} = V$ between sites 4 and 5. We call the (4,5) pair a dimer. The unperturbed system ($\epsilon = 0$) is integrable, since it decomposes into a DNLS dimer and 3 uncoupled single sites 1, 2 and 3 with conserved occupation probabilities. We are interested in the effect of the small couplings introduced by the ϵ–perturbing part of (2.1).

Introducing action–angle variables, Hamiltonian (2.1) becomes (see Appendix A)

$$H = H_d^0(x,y) + \sum_{j=1}^{3}(-\frac{\gamma}{8}(I_j + \hat{I}_j)^2) + \epsilon H^1(x, y, I_1, I_2, I_3, \psi_1, \psi_2, \psi_3, \mu) \tag{2.2}$$

where

$$H_d^0(x, y; N, \beta) = -\frac{\gamma}{4}(N^2 + x^2) - W_{45}\sqrt{N^2 - x^2}cosy \tag{2.3a}$$

$$H^1 = -\{\sum_{k=2}^{3} W_{1k}\sqrt{(I_1 + \hat{I}_1)(I_k + \hat{I}_k)}cos(\psi_1 - \psi_k) + W_{23}\sqrt{(I_3 + \hat{I}_3)(I_2 + \hat{I}_2)}cos(\psi_2 - \psi_3)$$

$$+ \sum_{j=1}^{3}[W_{4j}\sqrt{(N + x)(I_j + \hat{I}_j)}cos(\frac{y}{2} - \psi_j) + W_{5j}\sqrt{(N - x)(I_j + \hat{I}_j)}cos(\frac{y}{2} + \psi_j)]\} \tag{2.3b}$$

$\hat{\psi}_j$ are cyclic variables for the Hamiltonian and $N = \sum_{j=1}^{3} \hat{I}_j - P$. Thus, the reduced Hamiltonian (2.2) describes a 4 d.o.f system, whose equation of motion can be written as follows:

$$\dot{x} = -2V\sqrt{N^2 - x^2}siny + \epsilon\frac{\partial H^1}{\partial y} \quad \dot{y} = -\gamma x + \frac{2Vx}{\sqrt{N^2 - x^2}}cosy - \epsilon\frac{\partial H^1}{\partial x}$$

$$\dot{I}_j = -\epsilon\frac{\partial H^1}{\partial \psi_j} \quad \dot{\psi}_j = \frac{\partial H^0}{\partial I_j} + \epsilon\frac{\partial H^1}{\partial I_j} \tag{2.4}$$

with $j = 1, 2, 3$, $0 < \epsilon \ll 1$, $(x, y, I_1, I_2, I_3, \psi_1, \psi_2, \psi_3) \in \mathbb{R}^2 \times \mathbb{R}^3 \times T^3$

3. THE DNLS PENTAMER AND MEL'NIKOV 'S ANALYSIS

Let $\hat{V} \subset \mathbb{R}^2 \times \mathbb{R}^3$ and $W \subset \mathbb{R}^2 \times \mathbb{R}^3 \times \mathbb{R}^\rho$ be open sets the functions

$$H^0 : \hat{V} \longrightarrow \mathbb{R} \quad H^1 : W \times T^3 \longrightarrow \mathbb{R} \tag{3.1}$$

are defined and $\mathcal{C}^{r+1}$ $r > 8$.

The unperturbed system ($\epsilon = 0$) of (2.4) has a hyperbolic saddle fixed point at $(x, y) = (0, 0)$ for $\beta = \frac{N\gamma}{2V} > 1$. The coordinates of the homoclinic orbit associated with this saddle point for $2 > \beta > 1$, are given by:

$$x^{\pm}(t) = \pm x(t) = \frac{4V\sqrt{\beta - 1}}{\gamma}sech(2\sqrt{\beta - 1}Vt) \tag{3.2a}$$

$$y^{\pm}(t) = y(t) = arccos(\frac{N - \frac{\gamma x^2}{4V}}{\sqrt{N^2 - x^2(t)}}) \tag{3.2b}$$

For $\beta > 1$, the unperturbed system ($\epsilon = 0$) of (2.4) has a $\mathcal{C}^r$ 6–dimensional (6–D) normally hyperbolic invariant manifold

$$\mathcal{M}_0 = \{(\mathbf{x}, I, \psi) \in \mathbb{R}^2 \times \mathbb{R}^3 \times T^3 : \mathbf{x} = 0, I \in U \subset \mathbb{R}^3, \psi \in T^3\}$$

Moreover, $\mathcal{M}_0$ has $\mathcal{C}^r$, 7–D stable and unstable manifolds denoted $W^s(\mathcal{M}_0)$ and $W^u(\mathcal{M}_0)$, respectively which intersect along the 7–D homoclinic manifold

$$\Gamma^{\pm} = \{(x^{\pm}(-t_0), y^{\pm}(-t_0), I, \psi^0) \in \mathbb{R}^2 \times U \times T^3\} \tag{3.3}$$

cf (3.2). The unperturbed vector field restricted to $\mathcal{M}_0$ is described by the equations

$$\dot{\mathbf{I}} = 0 \quad \dot{\psi}_j = -\frac{\gamma}{4}(I_j + \hat{I}_j) \quad j = 1, 2, 3 \tag{3.4}$$

with the flow given by

$$I_j(t) = \bar{I}_j(0) \quad \psi_j(t) = -\frac{\gamma}{4}(\bar{I}_j + \hat{I}_j)t + \psi_j^0 \quad j = 1, 2, 3 \tag{3.5}$$

So $\mathcal{M}_0$ has the structure of an 3–parameter family of 3–tori, with the flow on the tori being either rational or irrational. For a fixed $\bar{I} \in U \subset \mathbb{R}^3$ the corresponding 3–torus on $\mathcal{M}$ is :

$$\tau(\bar{I}) = \{(x, I, \psi) \in \mathbb{R}^2 \times U \times T^3 : x = 0, I = \bar{I}\}$$

$\tau(\bar{I})$ has 4–D stable and unstable manifolds $W^{s,u}(\tau(\bar{I}))$ which intersect along 4D homoclinic manifold given by

$$\Gamma_I^{\pm} = \{(x_I^{\pm}(-t_0), y_I^{\pm}(-t_0), \bar{I}, \psi^0) \in \mathbb{R}^2 \times \mathbb{R}^3 \times T^3\}$$

Additionally, $\tau(\bar{I})$ has a 3 dimensional center manifold corresponding to the exponentially expanding or contacting directions tangent to $\mathcal{M}$.

For each $I \in U$, consider the following vector in $\mathbb{R}^2 \times \mathbb{R}^3 \times \mathbb{R}^3$:

$$\{(D_x H, 0)\}$$

where "0" denotes the 6-D zero vector. We define a set of 3 linearly indepedent constant unit vectors in $\mathbb{R}^2 \times \mathbb{R}^3 \times \mathbb{R}^3$

$$\{\check{I}_1, \ldots, \check{I}_3\}$$

where the $\check{I}_i$ represent unit vectors in I_i directions. We let $p = (x_I^{\pm}(-t_0), y_I^{\pm}(-t_0), \bar{I}, \psi^0)$ denote the corresponding point on Γ. Then Π_p is defined to be the 4–D plane spanned by the above 4 linearly independent vectors, where $D_x H$ is evaluated at p and the $\hat{I}_i$ are viewed as emanating from p. Hence, $W^{s,u}(\mathcal{M}) \cap \Pi_p = S_p^{s,u}$, is a 3–D manifold for each $p \in \Gamma$.

Clearly, the manifold $\mathcal{M}_0$ persists for sufficiently small $\epsilon \neq 0$, as a locally invariant 6D manifold $\mathcal{M}_\epsilon$ in the perturbed system and has local $\mathcal{C}^r$ stable and unstable manifolds $W^{s,u}(\mathcal{M}_\epsilon)$ close to $W^{s,u}(\mathcal{M}_0)$ [17].

The unperturbed vector field restricted to $\mathcal{M}_0$ is given by (3.4). Thus, (3.4) has the form of a 3 d.o.f completely integrable Hamiltonian system where I_j are integrals of motion and the entire phase space $U \times T^3$ is foliated by a 3–parameter family of 2-D tori with the three frequencies on the tori given by $-\frac{\gamma}{4}(\bar{I}_j + \hat{I}_j) \quad j = 1, 2, 3$.

Furthermore, under the assumption of nondegeneracy for the frequencies of the uncoupled oscillators,

$$det D_I^2 H^0(I) \neq 0 \quad (D_I^2 \equiv Hessian)$$

the KAM theorem can be invoked to conclude that for sufficiently small ϵ most of the nonresonant 3–tori are preserved. For fixed actions $\bar{\mathbf{I}}$, a 3-D invariant torus $\tau_\epsilon(\bar{\mathbf{I}})$ is located on $\mathcal{M}_\epsilon$. The existence of 4-D stable and unstable manifolds of the torus is guaranteed by virtue of Graff 's theorem.

To determine whether the $W^s(\tau_\epsilon(\bar{\mathbf{I}}))$ and $W^u(\tau_\epsilon(\bar{\mathbf{I}}))$ of the torus intersect on $\mathcal{M}_\epsilon$ transversely, we have to compute the distance d_ϵ between the local stable and unstable manifold at points along the unperturbed homoclinic orbits $\Gamma_I^{\pm}$.

Now the three components of the Mel'nikov vector

$$\mathbf{M}_{\bar{I}}(\psi_1^0, \psi_2^0, \psi_3^0) = (M_1(\psi_1^0), M_2(\psi_2^0), M_3(\psi_3^0)) \tag{3.6}$$

are proportional to the signed distances between $W^s(\tau_\epsilon(\bar{\mathbf{I}}))$ and $W^u(\tau_\epsilon(\bar{\mathbf{I}}))$, is determined, to order ϵ by, $(I_\epsilon^u)_j - (I_\epsilon^s)_j \quad j = 1,2,3$

According to Wiggins [13], the components of the Mel'nikov vector are given by the following three Mel'nikov integrals

$$M_j^{\pm}(\psi_j^0) = -\int_{-\infty}^{\infty} D_{\psi_j} H^1(x^{\pm}(t), y(t), \bar{I}, \psi_j(t) + \psi_j^0)\, dt \quad j = 1,2,3 \tag{3.7}$$

which is evaluated along the homoclinic orbit (3.2). We finally find, after some computations (see Appendix B)

$$M_j^+(\psi_j^0) = F_j(\bar{I}, \gamma, V, W_{4i}, W_{5j}) cos(\psi_j^0) + G_j(\bar{I}, \gamma, V, W_{4i}, W_{5j}) sin(\psi_j^0) \quad j = 1,2,3 \tag{3.8}$$

where F_j, G_j are functions of the system parameters determined via convergent integrals as explained in Appendix B.

¿From the above, it is clear that the components of the Mel'nikov vector have *simple zeros* at

$$\psi_j^0 = arctan(-\frac{F_j}{G_j}) + k\pi, \quad k \in Z \tag{3.9}$$

and since

$$rank\{D_{(\psi_1^0, \psi_2^0, \psi_3^0)} \mathbf{M}_{\bar{I}}(\psi_1^0, \psi_2^0, \psi_3^0)\} = 3 \tag{3.10}$$

where

$$D_{\psi^0} \mathbf{M}_{\bar{I}}(\psi^0) = \begin{pmatrix} \frac{\partial \mathbf{M}_{\bar{I}}^+}{\partial \psi_1} & \frac{\partial \mathbf{M}_{\bar{I}}^+}{\partial \psi_2} & \frac{\partial \mathbf{M}_{\bar{I}}^+}{\partial \psi_3} \\ \frac{\partial^2 \mathbf{M}_{\bar{I}}^+}{\partial \psi_1^2} & \frac{\partial^2 \mathbf{M}_{\bar{I}}^+}{\partial \psi_2 \psi_1} & \frac{\partial^2 \mathbf{M}_{\bar{I}}^+}{\partial \psi_2^2} \end{pmatrix} \quad or \quad \begin{pmatrix} \frac{\partial \mathbf{M}_{\bar{I}}^+}{\partial \psi_1} & \frac{\partial \mathbf{M}_{\bar{I}}^+}{\partial \psi_2} & \frac{\partial \mathbf{M}_{\bar{I}}^+}{\partial \psi_3} \\ \frac{\partial^2 \mathbf{M}_{\bar{I}}^+}{\partial \psi_1 \psi_2} & \frac{\partial^2 \mathbf{M}_{\bar{I}}^+}{\partial \psi_2^2} & \frac{\partial^2 \mathbf{M}_{\bar{I}}^+}{\partial \psi_2 \psi_3} \end{pmatrix} \tag{3.11}$$

the stable and unstable manifolds, $W^{s,u}(\tau_\epsilon(\bar{I}))$ of the KAM torus intersect transversely near (ψ_1^0, ψ_2^0, ψ_3^0) in the 7–D energy surface.

Summarizing, let us note that, in the $\epsilon = 0$ case, we have started, on a fixed 7–D energy manifold with a two parameter family of 3–tori. Each such torus has 4–D stable and unstable manifolds which coincide along a 4–D homoclinic orbit, while the tori (along with their stable and unstable manifolds) are not isolated on the energy manifold. In the perturbed system, most of this 2 parameter family of tori survive and their stable and unstable manifolds intersect transversely. In particular the unstable manifold of $\tau_\epsilon(I_2)$, transveresly intersects $W^s(\tau_\epsilon(\bar{I}_3))$and $W^s(\tau_\epsilon(\bar{I}_1))$, which are arbitrarily close. The resulting tangle of manifolds provides a mechanism through which orbits may wander in an apparently chaotic fashion amongst the KAM tori.

If we now substitute on the right hand side of equations (2.4a)

$$(x(t), y(t), I_j(t), \psi_j(t)) = (x^{\pm}(t) + \mathcal{O}(\epsilon), y^{\pm}(t) + \mathcal{O}(\epsilon), \bar{I}_j + \epsilon I_j^{(1)} + \mathcal{O}(\epsilon^2), -\frac{\gamma}{4}(\bar{I}_j + \hat{I}_j)t + \psi_j^0 + \mathcal{O}(\epsilon))$$

and integrate from $-\infty$ to ∞ we have after some algebra

$$\Delta I_j^{(1)} = \frac{1}{\sqrt{2}}\{M_j^{\pm}(\psi_j^0) - [C(\bar{I}, \gamma, V, W_{4j}, W_{5j}) cos(\psi_j^0) + D(\bar{I}, \gamma, V, W_{4j}, W_{5j}) sin(\psi_j^0)]\}$$

$$C := \sqrt{\bar{I}_j + \hat{I}_j} \int_{-\infty}^{\infty} sin\omega_j t[W_{5j} S_+ T_- + W_{4j} S_+ T_+]\, dt$$

and

$$D := -\sqrt{\bar{I}_j + \hat{I}_j} \int_{-\infty}^{\infty} sin\omega_j t[W_{5j} S_- T_- - W_{4j} S_- T_+]\, dt$$

$S_\pm$, $T_\pm$ are as defiuned in Appendix B.

We now want to describe how the transport via lobes of this homoclinic tangle is related to Arnold diffusion. The geometry of transport in phase space has been studied by Rom–Kedar and Wiggins [16]. The normally hyperbolic invariant maniifold $\mathcal{M}$ has the structure of 3-parameter family of 3–D tori denoted by $\tau(I)$, where each torus has an 4–D stable and unstable manifolds, and a 6–D center manifold. For the unparturbed system these tori, along with their invariant manifolds are not isolated. Now, when the system is perturbed, a generalization of the KAM theorem due to Graff tell us that a Cantor set of tori on $\mathcal{M}$, having positive meausure, is preserved. At the same time, generically the stable and unstable manifolds of these tori will intersect transverely, yielding a homoclinic tangle. Near the torus, the homoclinic tangle exhibits large amplitude oscillations due to the hyperbolicity. Since we have a Cantor set such tori, this set is dense in itself, therefore the homoclinic tangle of each torus becomes intertwined with the homoclinic tangles of nearby tori leading to the possibility that orbits, starting near any one of these tori, may *diffuse* along this Cantor set of homoclinic tangles in a chaotic fushion. This situation was first described by Arnold [2] and has come to be known as *Arnold diffusion*; it can be verified for our DNLS pentamer, using Melnikov-type arguments described before. Arnold diffusion occurs in the I variables (along directions "tangent" to $W^s(\mathcal{M})$ and $W^u(\mathcal{M})$) and transport via lobes occurs in the x directions (along directions transverse to $W^s(\mathcal{M})$ and $W^u(\mathcal{M})$).

4. THE N–ELEMENTS DNLS SYSTEM

In this section we generalize the results of section 3 and study the N–element DNLS and proving the existence of chaotic solutions. Now, the DNLS N–mer Hamiltonian, in terms of the complex site occupation amplitude, can be written as:

$$H = -\frac{1}{2}\gamma \sum_{j=1}^{N} |c_j|^4 - W_{N-1,N}(c^*_{N-1}c_N + c^*_N c_{N-1}) - \epsilon \sum_{k=1}^{N-2} \sum_{j=k+1}^{N} W_{kj}(c^*_k c_j + c^*_j c_k) \tag{4.1}$$

The assumptions of the case $N = 5$ of section 3 still hold, and the correspoding dimer integrable system is defined here by the pair $(N-1, N)$, and

$$P = \sum_{j=1}^{N} |c_j|^2 \tag{4.2}$$

is a conserved quantity. Let us write the Hamiltonian (4.1) in a different form resulting from (see Appendix A)

- a transformation of $c_1, \cdots, c_{N-2}$ to action–angle variables

$$c_j = \sqrt{J_j} e^{-i\theta_j} \tag{4.3}$$

- a symplectic transformation of the dimer amplitudes c_{N-1}, c_N to two pairs of canonically–conjuagate variables (x, y) and (L, β):

$$c_{N-1} = \sqrt{\frac{L+x}{2}} e^{-i(\frac{y}{2}+\beta)} \quad c_N = \sqrt{\frac{L-x}{2}} e^{i(\frac{y}{2}-\beta)} \tag{4.4}$$

and

$$x = |c_{N-1}|^2 - |c_N|^2 \quad L = |c_{N-1}|^2 + |c_N|^2$$

$$P = \sum_{j=1}^{N-2} J_j + L$$

Thus, the unperurbed Hamiltonian becomes:

$$H_0 = -\frac{\gamma}{2} \sum_{j=1}^{N-2} J_j^2 - \frac{\gamma}{4}(L^2 + x^2) - W_{N-1,N}\sqrt{L^2 - x^2} cosy \tag{4.5}$$

while the interaction Hamiltonian is given by:

$$H_1 = -\{\sum_{k=1}^{N-2}\sum_{j=k+1}^{N-2} 2W_{kj}cos(\theta_j - \theta_k)+$$

$$\sum_{j=1}^{N-2}[W_{N-1,j}\sqrt{2(L+x)J_j}cos(\frac{y}{2}+\beta-\theta_j) + W_{N,j}\sqrt{2(L-x)J_j}cos(\frac{y}{2}+\beta+\theta_j) \tag{4.6}$$

The original complex variables c_j span the $2N$ dimensional product space of $\mathbb{C}$, which reduces to dimension of $2N-2$, as a result of the two conserved quantities H and P.

We introduce, as before, new couples of canonically conjuagate action–angle variables (I_j, ψ_j) and $\hat{I}_j, \hat{\psi}_j)$ with the generating function

$$F = \sum_{j=1}^{N-2}[(\theta_j - \beta)I_j + (\theta_j + \beta)\hat{I}_j] \tag{4.7}$$

whence the Hamiltonian (4.5), (4.6) become:

$$H_0 = H_d^0 + \sum_{j=1}^{N-2}(-\frac{1}{8}(I_j + \hat{I}_j)^2) \tag{4.8}$$

and

$$H_1 = -\{\sum_{k=1}^{N-2}\sum_{j=k+1}^{N-2} W_{kj}\sqrt{(I_k+\hat{I}_k)(I_j+\hat{I}_j)}cos(\psi_j - \psi_k)+$$

$$\sum_{j=1}^{N-2}[W_{N-1,j}\sqrt{(L+x)(I_j+\hat{I}_j)}cos(\frac{y}{2}-\psi_j) + W_{N,j}\sqrt{(L-x)(I_j+\hat{I}_j)}cos(\frac{y}{2}+\psi_j) \tag{4.9}$$

$\hat{\psi}_j$ are cyclic variables. The reduced Hamiltonian system (4.8), (4.9) has $(N-1)$–d.o.f and can be written in a similar form as (2.4), where $(x, y, I, \psi) \in \mathbb{R}^2 \times \mathbb{R}^{N-2} \times T^{N-2}$.

Finally, the $N-2$ components of the Mel'nikov vector are given by the following formula:

$$M_j^+ = F_j(\bar{I}, \gamma, V, W_{N-1,j}, W_{N,j})cos(\psi_j^0) + G_j(\bar{I}, \gamma, V, W_{N-1,j}, W_{N,j})sin(\psi_j^0) \tag{4.10}$$

see (3.8). The components of the Mel'nikov vector have simple zeros at

$$\psi_j^0 = tan^{-1}(-\frac{F_j}{G_j}) + \lambda\pi \tag{4.11}$$

and since

$$rankD_\psi \mathbf{M}_I^+(\psi^0) = N-2$$

the stable and unstable manifolds of the KAM torus intersect transversely near $(\psi_1^0, \cdots, \psi_{N-2}^0)$ in the $(2N-3)$ dimensional energy surface.

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APPENDIX A

We define the total "momentum"

$$P = \sum_{j=1}^{5} |c_j|^2 \tag{A1}$$

which is a conserved quantity for the DNLS system (1.1), with $n = 5$. Let us write the Hamiltonian (2.1) in a different form resulting from:

- a transformation of c_1, c_2, c_3 to action–angle variables

$$c_j = \sqrt{J}_j e^{-i\theta_j}, \qquad j = 1, 2, 3 \tag{A2}$$

- a symplectic transformation of the dimer amplitudes c_4, c_5 to 2 pairs of (real) canonically–conjuagate variables (x, y) and (N, β)

$$c_4 = \sqrt{\frac{N+x}{2}} e^{-i(\frac{y}{2}+\beta)} \tag{A3a}$$

$$c_5 = \sqrt{\frac{N-x}{2}} e^{i(\frac{y}{2}-\beta)} \tag{A3b}$$

where $x = |c_4|^2 - |c_5|^2$, $N = |c_4|^2 + |c_5|^2$ and

$$P = \sum_{j=1}^{3} J_j + N$$

Now the Hamiltonian (2.1) can be written in the form:

$$H = H_d^0(x, y; N, \beta) + \sum_{j=1}^{3} H_j^0(J_j) + \epsilon H^1(x, y, N, \beta, J_1, J_2, J_3, \theta_1, \theta_2, \theta_3) \tag{A4}$$

where

$$H_d^0(x, y; N, \beta) = -\frac{\gamma}{4}(N^2 + x^2) - W_{45}\sqrt{N^2 - x^2}cosy$$

$$H_j^0(J_j) = -\frac{1}{2}\gamma J_j^2$$

and

$$H^1 = -\{2W_{12}\sqrt{J_1 J_2}cos(\theta_2 - \theta_1) + 2W_{13}\sqrt{J_1 J_3}cos(\theta_3 - \theta_1) + 2W_{23}\sqrt{J_2 J_3}cos(\theta_2 - \theta_3)$$
$$+\sum_{j=1}^{3}[W_{4j}\sqrt{2(N + x)J_j}cos(\frac{y}{2} + \beta - \theta_j) + W_{5j}\sqrt{2(N - x)J_j}cos(\frac{y}{2} - \beta - \theta_j)]\}$$

The original complex variables c_j span the 10 dimensional product space, which reduces to 8 dimensions as a result of the two conserved quantities H and P.

Note that the interaction Hamiltonian depends on the angle variables β and $\theta_j, j = 1, 2, 3$ only through their combination $(\theta_j - \beta)$, which suggests passing to new angle variables $\psi_j = (\theta_j - \beta)$ and then to new couples of canonically conjuagate action–variables (I_j, ψ_j) and $(\hat{I}_j, \hat{\psi}_j)$ using the generating function

$$F = \sum_{j=1}^{3}[(\theta_j - \beta)I_j + (\theta_j + \beta)\hat{I}_j] \tag{A5}$$

Using these transformations the iteraction Hamiltonian H^1 finally assumes the from given in (2.3b).

APPENDIX B

The goal of this Appendix is to outline the proof of equation (3.8). We have:

$$M_j^+ = -\sqrt{\bar{I}_j + \hat{I}_j}\int_{-\infty}^{\infty}[W_{5j}(S_-(t)cos(\psi_j^0) + S_+(t)sin(\psi_j^0))T_-(t) - W_{4j}(S_-(t)cos(\psi_j^0)$$
$$-S_+(t)sin(\psi_j^0))T_+(t)]cos(\omega_j t)\,dt + (-1)^j[W_{12}\sqrt{(\bar{I}_1 + \hat{I}_1)(\bar{I}_2 + \hat{I}_2)}\int_{-\infty}^{\infty} sin(\omega_{12}t + (\psi_1^0 - \psi_2^0))\,dt$$
$$+\sum_{k=1}^{2} W_{k3}\sqrt{(\bar{I}_k + \hat{I}_k)(\bar{I}_3 + \hat{I}_3)}\int_{-\infty}^{\infty} sin(\omega_{k3}t + (\psi_3^0 - \psi_k^0))\,dt] \tag{B1}$$

with

$$S_\pm = \sqrt{\sqrt{N^2 - x^2(t)} \pm (N - \frac{\gamma}{4V}x^2(t))} \tag{B2.a}$$

$$T_\pm = \Big(\frac{N \pm x(t)}{N \mp x(t)}\Big)^{1/4} \tag{B2.b}$$

$$\omega_j = \frac{\gamma}{4}(\bar{I}_j + \hat{I}_j) \tag{B2.c}$$

$$\omega_{12} = -\frac{\gamma}{4}((\bar{I}_1 - \bar{I}_2) + (\hat{I}_1 - \hat{I}_2)) \tag{B2.d}$$

$$\omega_{k3} = -\frac{\gamma}{4}((\bar{I}_k - \bar{I}_3) + (\hat{I}_k - \hat{I}_3)) \quad k = 1, 2 \qquad (B2.d)$$

We therefore consider the improper integrals as the following limit of a sequence in time:

$$\tau_n^{s,u} = \pm\frac{2\pi n}{\omega_j} \quad j = 1, 2, 3$$

$$M_j^+ = -\lim_{n\to\infty}\sqrt{\bar{I}_j + \hat{I}_j}\int_{-\frac{2\pi n}{\omega_j}}^{\frac{2\pi n}{\omega_j}}[W_{5j}(S_-(t)cos(\psi_j^0) + S_+(t)sin(\psi_j^0))T_-(t) - W_{4j}(S_-(t)cos(\psi_j^0)$$

$$-S_+(t)sin(\psi_j^0))T_+(t)]cos(\omega_j t)\,dt + (-1)^j[W_{12}\sqrt{(\bar{I}_1 + \hat{I}_1)(\bar{I}_2 + \hat{I}_2)}$$

$$\lim_{n\to\infty}\int_{-\frac{2\pi n}{\omega_{12}}}^{\frac{2\pi n}{\omega_{12}}} sin(\omega_{12}t + (\psi_1^0 - \psi_2^0))\,dt$$

$$+\sum_{k=1}^{2} W_{k3}\sqrt{(\bar{I}_k + \hat{I}_k)(\bar{I}_3 + \hat{I}_3)}\lim_{n\to\infty}\int_{-\frac{2\pi n}{\omega_{k3}}}^{\frac{2\pi n}{\omega_{k3}}} sin(\omega_{k3}t + (\psi_3^0 - \psi_k^0))\,dt] \qquad (B3)$$

Finally we have:

$$M_j^+(\psi_j^0) = -[F_j(\bar{I}, \gamma, V, W_{4j}, W_{5j})cos(\psi_j^0) + G_j(\bar{I}, \gamma, V, W_{4j}, W_{5j})sin(\psi_j^0)] \qquad (B4)$$

where F_j, G_j are functions of the system parameters determined via the integrals

$$F := \sqrt{\bar{I}_j + \hat{I}_j}\int_{-\infty}^{\infty} cos\omega t[W_{5j}S_-T_- - W_{4j}S_-T_+]\,dt$$

$$G := \sqrt{\bar{I}_j + \hat{I}_j}\int_{-\infty}^{\infty} cos\omega t[W_{5j}S_+T_- + W_{4j}S_+T_+]\,dt$$

as $n \longrightarrow \infty$.