Chaos in a Near–Integrable Hamiltonian Lattice*

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Abstract

We study the chaotic dynamics of a near–integrable Hamiltonian Ablowitz-Ladik lattice, which is $N + 2$-dimensional if $N$ is even ($N + 1$ if $N$ is odd) and possesses, for all $N$, a circle of unstable equilibria at $\varepsilon = 0$, whose homoclinic orbits are shown to persist for $\varepsilon \neq 0$ on whiskered tori. The persistence of homoclinic orbits is established through Mel’nikov conditions, directly from the Hamiltonian structure of the equations. Numerical experiments which combine space portraits and Lyapunov exponents are performed for the perturbed Ablowitz-Ladik lattice and large scale chaotic behavior is observed in the vicinity of the circle of unstable equilibria of the $\varepsilon = 0$ case. We conjecture that this large scale chaos is due to the occurrence of saddle–center type fixed points in a perturbed 1 d.o.f Hamiltonian to which the original system can be reduced for all $N$. As $\varepsilon > 0$ increases, the transient character of this chaotic behavior becomes apparent as the positive Lyapunov exponents steadily increase and the orbits escape to infinity.

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1 Introduction

Homoclinic orbits of dynamical systems are important in applications for a number of reasons, one of them being that they often form ‘organizing centers’ for the dynamics in their neighborhood. From their existence and intersection one may, under certain conditions, infer the existence of chaos nearby e.g. using shift dynamics associated with Smale horseshoes [Shi'nikov, 1965 and Smale, 1967].

Mel'nikov’s method is one of the few analytical tools which can be used to detect, in the context of perturbation theory, the splitting and intersection of homoclinic manifolds. It has the nice geometrical interpretation that it can provide a measure of the projection of the splitting distance onto a direction normal to the unperturbed level sets. A discussion of the generalization of the original ideas of Mel’nikov to many dimensions can be found e.g. in [Wiggins, 1988].

The present paper deals with a class of multi-degree-of-freedom dynamical systems which arise as spatial discretizations of a partial differential equation on the periodic domain. In particular, we consider the integrable discretization of the nonlinear Schrödinger equation (NLS), Ablowitz-Ladik (AL) lattice, with a conservative type of perturbation also considered by [Li, 1998]:

\[ i\dot{q}_n = \frac{q_{n+1} - 2q_n + q_{n-1}}{\hbar^2} + |q_n|^2(q_{n+1} + q_{n-1}) - 2\omega^2q_n + \varepsilon \left[ a_1(q_n^2 + |q_n|^2) + a_2(q_n^2 + |q_n|^2)q_n + (a_1 + 2a_2\bar{q}_n)\frac{\rho_n}{\hbar^2}|\rho_n| \right] \]

(1)

where \( q_n \) are complex variables, \( \rho_n := 1 + \hbar^2|q_n|^2, \ h = 1/N, \ n = 0, 1, \ldots, N - 1, \ \omega, \ a_1, \ a_2 \) are real constants and \( \varepsilon \) is a small parameter. We assume that system (1) satisfies the following even periodic boundary conditions

\[ q_{N+n}(t) = q_n(t), \quad q_{N-n}(t) = q_n(t) \]

and its phase space is defined as:

\[ \mathcal{N} = \left\{ (q, r) : r = -\bar{q}, \ q = (q_0, \ldots, q_{N-1}), \ q_{N+n} = q_n, \ q_{N-n} = q_n \right\} \]

(2)

Equation (1) is a \( 2(M + 1) \)-dimensional system, where \( M = N/2 \), if \( N \) is even, \( M = (N-1)/2 \), if \( N \) is odd which is known to be integrable for \( \varepsilon = 0 \) with Hamiltonian formulation and a corresponding Lax pair.

First, we establish necessary conditions for the persistence of homoclinic orbits in Ablowitz-Ladik lattices with Hamiltonian perturbations. The Mel'nikov conditions are derived directly from the Hamiltonian structure of the equations via the averaging method. The unperturbed system has finite dimensional whisker tori (hyperbolic invariant tori), with coincident whiskers (invariant manifolds), while Mel'nikov's method allows us to study the splitting of whiskers and the persistence of homoclinic orbits. The homoclinic splitting between the whiskers of hyperbolic tori is very important for the study of diffusion of orbits in phase space.

We have also carried out numerical calculations associated with the near-integrable Hamiltonian AL-lattice (1) with periodic boundary conditions. It is well known that equation (1) (for \( \varepsilon = 0 \)), as well as its continuum limit, have solutions which are linearly unstable and are associated with interesting mathematical and physical properties. Our numerical experiments through the calculation of Lyapunov exponents and phase portraits indicate the existence of large scale chaotic behavior near certain resonances, when \( \varepsilon \neq 0 \). We investigate this chaotic dynamics for the specific perturbation given in (1) for special values of the external parameters satisfying Mel'nikov conditions and observe the phenomenon of transient chaos, through which, for \( \varepsilon \) large enough orbits escape to infinity.

Other researchers, [Li & McLaughlin, 1997], [Haller, 1998] have also studied persistence questions related to discrete nonlinear Schrödinger (DNLS) equations. Their type of perturbations, however, is
dissipative and hence different from the one adopted here. Recently, Li [1998] proved the existence of transversal homoclinic tubes which are asymptotic to locally invariant center manifolds for the DNLS with Hamiltonian perturbations. Ablowitz & Herbst [1990] were concerned with the question of numerical instability involving periodic NLS equations. They showed that initial data which are near low-dimensional homoclinic manifolds trigger numerically induced joint spatial and temporal chaos in non-integrable numerical schemes at intermediate values of the mesh size $h$. This type of chaos disappears as the mesh is refined [Hersht & Ablowitz, 1989]. Furthermore, the presence of homoclinic orbits in DNLS-type systems has been studied by [Kollman & Bountis, 1998] who used different methods, based on the homoclinic bifurcations of finite dimensional reduced mappings.

The present paper is organized as follows: In section 2, we formulate the Hamiltonian structure of the problem and the geometry of the perturbed system. In section 3, we derive necessary criteria for the persistence of homoclinic orbits and in section 4, we present numerical evidence showing that the perturbed system (1) indeed possesses large scale chaotic dynamics near some fundamental resonances of the system, identified by the analysis of section 2 and 3.

2 Hamiltonian Structure and Geometry

2.1 The geometry of the unperturbed system

In this section, we give a brief overview of the integrable AL lattice and its homoclinic structure. Eq. (1), for $\varepsilon = 0$, together with the equation of its complex conjugate variables $\tilde{q}_n$, possess the Hamiltonian formulation:

$$H_0 = \frac{1}{\hbar^2} \sum_{n=1}^{N-1} \left[ \tilde{q}_n (q_{n+1} + q_{n-1}) - \frac{2}{\hbar^2} (1 + \omega^2 \hbar^2) \log(1 + \hbar^2 |q_n|^2) \right],$$

with the deformed Poisson brackets

$$\{q_n, \tilde{q}_m\} = i(1 + \hbar^2 |q_n|^2)\delta_{nm}, \quad \{q_n, q_m\} = \{\tilde{q}_n, \tilde{q}_m\} = 0,$$

and the symplectic form

$$\Omega = \sum_{n=0}^{N-1} \frac{i}{2(1 + \hbar^2 |q_n|^2)} \text{Im}(d\tilde{q}_n \wedge dq_n),$$

where we have defined

$$\{B, C\} = i \sum_{n=1}^{N-1} \left( \frac{\partial B}{\partial \tilde{q}_n} \frac{\partial C}{\partial q_n} - \frac{\partial B}{\partial q_n} \frac{\partial C}{\partial \tilde{q}_n} \right) (1 + \hbar^2 |q_n|^2).$$

The integrability of the unperturbed equation is proven using the discretized Lax pair [Ablowitz & Ladik, 1976]:

$$u_{n+1} = L_n(z, q)u_n, \quad u_n = B_n(z, q)u_n$$

where $L_n, B_n$ are $2 \times 2$ matrices and $z = \exp(i \lambda \hbar)$ is the spectral parameter of the problem.

In the case of periodic boundary conditions, let $Y^{(1)}, Y^{(2)}$ be the fundamental solutions of eq. (4). The associated Floquet discriminant is defined by

$$\Delta : \mathbb{C} \times \mathcal{N} \to \mathbb{C}, \quad \Delta(z, q) = \text{trace} \{M_q(N, z; q)\}$$

where $\mathcal{N}$ is the phase space defined in (2) and $M(n, z, q) \equiv \text{columns}\{Y^{(1)}_n, Y^{(2)}_n\}$ is the fundamental solution matrix of eqs. (4).
Following Li [1992], the Floquet theory is not standard as can be seen from the Wronskian relation:

\[ W_N(u^+, u^-) = D^2 W_0(u^+, u^-), \quad D^2 = \prod_{n=0}^{N-1} \left( 1 + h^2 |q_n|^2 \right) \]

where \( u^+ \) and \( u^- \) are any two solutions to the linear system (4). The nonstandard Floquet theory for integrable lattices (discrete systems in space and time) is established by Rothos [2001]. The Floquet spectrum is defined as the closure of the complex \( z \) for which there exists a bounded eigenfunction to (4). In terms of the Floquet discriminant \( \Delta \), this is given by

\[ \sigma(L_n) = \left\{ \ z \in \mathbb{C} : -2D \leq \Delta(z; q) \leq 2D \right\} \]

Periodic and antiperiodic points \( z^\pm \) are defined by

\[ \Delta(z^\pm; q) = \pm 2D \]

A critical point \( z^c \) is defined by the condition

\[ \frac{d\Delta}{dz}(z^c; q) = 0 \]

An important sequence of constants of motion \( F_j \) for the unperturbed system is given in terms of the Floquet discriminant by Li [1998]

\[ F_j : C \subset \mathcal{N} \rightarrow \mathbb{C} \quad \text{with} \quad F_j = \frac{1}{D} \Delta(z_j; \ q) \quad (6) \]

where \( z^c \) be a simple critical point as defined above and \( \{ H_0, F_j \} = 0 \). These invariants \( F_j \)'s are candidate for building Melnikov functions.

We do not intend to discuss the homoclinic structure too deeply here (see Li [1992, 1998] for details). Due to the boundary conditions, the unperturbed integrable system (1) admits an invariant plane

\[ \Pi = \left\{ (q_i, -\bar{q}_i) \in \mathcal{N} : q_1 = q_2 = \ldots = q_N \right\} \]

of spatially independent solutions. Consider the uniform solution \( q_n = q, \ \forall n \) of the form

\[ q_n(t) = a \exp[-i \left( 2(a^2 - \omega^2)t - \varphi \right)], \quad (7) \]

where \( \varphi \) is a constant. We choose the amplitude \( a \) in the range: for \( N > 3 \ a \in (N \tan \frac{\pi}{N}, N \tan \frac{2\pi}{N}) \) and for \( N = 3 a > 3 \tan \frac{\pi}{3} \). The invariant plane \( \Pi \) contains the resonance circle

\[ \mathcal{N}_\omega = \left\{ (q_i, -\bar{q}_i) : |q_i| = \omega \right\} \]

entirely consists of fixed points under the unperturbed flow.

The hyperbolic structure and homoclinic orbits for the unperturbed system have been studied by Li [1992], using Birkhoff transformations, showing that, along the unstable and stable directions, solutions leave and return to the circle of equilibria \( \mathcal{N}_\omega \). This implies the existence of heteroclinic orbits in the phase space \( \mathcal{N} \) which connect different equilibria in \( \mathcal{N}_\omega \). From any point on the resonant circle \( \mathcal{N}_\omega \) there are precisely two homoclinic connections to another point of the circle. For the uniform solution (7), there is only one set of quadruplets of double points which are not on the unit circle and denote one of
them by $z = z^t_i = z^j_i$. For this reason, we consider in the following analysis only the first member of the sequence of invariants $F_j$. The heteroclinic solutions are of the form (Li, 1992)

$$Q_n(t) = q_c \left( \frac{E}{K_n} - 1 \right)$$

(8)

where

$$E = 1 + \cos 2\gamma - \sin 2\gamma \tanh \tau, \quad K_n = 1 \pm \frac{1}{\cos \theta} \sin \gamma \sech \tau \cos 2n \theta,$$

$$\tau = 4N^2 \sqrt{\rho \sin \theta \sqrt{\rho \cos^2 \theta - 1}} \cdot t - t_0, \quad \gamma = \tan^{-1} \frac{\sqrt{\rho \cos^2 \theta - 1}}{\sqrt{\rho \sin \theta}}, \quad \theta = \pi /N, \quad \rho = 1 + |q|^2 /N^2.$$

The index $\pm$ refers to two distinct families, which in turn are parameterized by the phase variable $\varphi$, and the initial time $t_0$. These orbit families form two, 2-dimensional homoclinic manifolds $W^\pm(\mathcal{N}_c)$ to $\mathcal{N}_c$.

Formula (8) also gives the two limit points of the heteroclinic connections

$$\lim_{t \to \pm \infty} Q_n(t) = a \exp \left[ \mp i \frac{\Delta \varphi}{2} \right]$$

(9)

where $\Delta \varphi$ is a constant phase shift between the limit points of every heteroclinic orbit

$$\Delta \varphi = -4 \tan^{-1} \frac{\sqrt{\rho \cos^2 \theta - 1}}{\sqrt{\rho \sin \theta}}$$

2.2 Geometry of the perturbed system

Usually, when we study a completely integrable Hamiltonian system with $n$ degrees of freedom (d.o.f) and Hamiltonian perturbation we use the action-angle formulation to derive the corresponding equations of motion. From the properties of the unperturbed system, we know that its phase space is foliated by a $k \leq n$-parameter family of $k$-tori. The tori can be either resonant or nonresonant. From the standpoint of perturbation theory, we are interested in what happens to this $k$-parameter family of tori under perturbation. Classical KAM theory is concerned with the persistence of $k$-dimensional diophantine tori under perturbation. Broadly speaking, there are two approaches for proving the persistence of $k$-dimensional tori on which the flow is quasiperiodic with diophantine frequencies: The global approach of Arnold and the local approach of Kolmogorov.

The crucial problem lies with the fate of the lower (i.e. $k \leq n$) dimensional tori. The KAM tori are elliptic in terms of their stability type. That is, they are neutrally stable in the linear approximation. For the low dimensional tori, there is also the possibility that they may have exponentially growing and contracting directions in the linear approximation, whence they are called whiskered tori. Graff [1974] has considered a “KAM-type” situation where the unperturbed problem has a submanifold foliated by invariant tori. Restricted to this submanifold, the dynamics is preserved and the preserved tori have stable and unstable manifolds. In our problem the situation is different: The unperturbed system has a circle of fixed points on a 2-dimensional manifold and each point on the circle of fixed points is connected to another fixed point on the circle by a heteroclinic orbit.

As we mentioned earlier, there exists a 2-dimensional manifold $\Pi \subset \mathcal{N}$ which is invariant under the flow of (1) for $\varepsilon = 0$ and is symplectic with the restricted nondegenerate two-form $\Omega_{\Pi} = \Omega |_{\Pi}$. Thus, for $\varepsilon = 0$, system (1) restricted to $\Pi$ becomes a 1 d.o.f completely integrable Hamiltonian system and the Liouville–Arnold–Jost theorem [ArnoF’d, 1978] guarantees the existence of an open set $\Pi$ on which we can introduce canonical action-angle variables $(I, \phi) \in \mathbb{R} \times S^1$. 

5
By restricting the flow to the invariant plane $\Pi$, one obtains a dimensional reduction of the system (1) for all $N$. This means that on $\Pi$ the equation of motion takes the following form:

$$i\dot{q} = 2(|\bar{q}|^2 - \omega^2)q + \varepsilon \left\{ a_1(q + \bar{q}) + a_2(q^2 + \bar{q}^2)|q| + \frac{a_1 + 2a_2}{\hbar^2} ln|\rho| \right\}$$

This shows that for $\varepsilon = 0$, $\Pi$ contains a circle of equilibria $\mathcal{N}_\omega$ given by

$$\mathcal{N}_\omega = \{ q : |q| = \omega \}$$

which is surrounded by periodic solutions (in the space $\Pi$) of the form (7), where the constant $\omega$ satisfies:

$$N \tan \frac{\pi}{N} < \omega < N \tan \frac{2\pi}{N}, \text{ if } N > 3, \quad \omega > 3 \tan \frac{\pi}{3}, \text{ if } N = 3$$

For any point $q \in \Pi$, there always exists an open neighborhood with local regular coordinates $I, \phi$, such that the symplectic form is written in the canonical form $\Omega|_\Pi = \sum dI_n \wedge d\phi_n$. Introducing now the amplitude-phase representation $(I, \phi) \in \mathbb{R} \times S^1$ in a neighborhood of $\Pi$ by writing $q = Ie^{i\phi}$, we obtain the equations of motion

$$\frac{dI}{dt} = -\varepsilon \sin(\phi(a_1 + 4a_2I\cos\phi))W_I$$

$$\frac{d\phi}{dt} = -2(I^2 - \omega^2) - \varepsilon \left\{ 2I(a_1\cos\phi + a_2I\cos2\phi) + \left( a_1\frac{\cos\phi}{I} + 2a_2\cos2\phi \right) W_I \right\}$$

(10)

where

$$W_I = \frac{1 + \hbar^2 I^2}{\hbar^2} \ln(1 + \hbar^2 I^2)$$

Thus, for $\varepsilon = 0$, system (1) restricted to $\Pi$ becomes a 1 d.o.f completely integrable Hamiltonian system.
Introducing the new scaling \( I = \omega + \sqrt{\varepsilon} J \) (which is just the standard blow-up transformation used in classical mechanics) to study the dynamics near a resonant action value and setting \( \sqrt{\varepsilon} = 0 \), we obtain a Hamiltonian system with

\[
\mathcal{H}(J, \phi) = 2\omega J^2 + W_\omega(a_1 \cos \phi + a_2 \omega \cos 2\phi) \quad := \frac{1}{2} \langle J, D^2 h_0(\omega) J \rangle + h_1(\phi)
\]

(11)

where \( h_0 := H_0|_\Pi \) is the restriction of \( H_0 \) to the manifold \( \Pi \) and \( h_1 = H_1|_{\mathcal{N}} \).

For \( a_1, a_2 > 0 \) and \( |a_1|/4a_2\omega < 1 \), the fixed points of the reduced system are \((0,0),(0,\pi)\) (saddle-type) and \((0,\pm \cos^{-1}(-a_1/4a_2\omega))\) (center-type). For \( a_1 > 0, |a_1|/4a_2\omega > 1 \), \((0,0)\) is a saddle point and \((0,\pi)\) center fixed point (see Fig. 1) below some of the orbits starting very close to the origin.

In order to provide a clearer geometric formulation for the problem, it is convenient to introduce local coordinates \( r = (r_u, r_v) \in \mathbb{R}^2, z \in \mathbb{R}^{2(M-1)} \), \((J, \phi) \in \mathbb{R} \times S^1 \) and \( r_c = (z, J, \phi) \), in a neighborhood of the set \( \mathcal{N}_c \) (see Li & McLaughlin [1997], Haller [1998]. Rothos [1999]) and the perturbed AL-lattice can be rewritten in the following form defined on the compact domain:

\[
\mathcal{Y} = \left\{ (r, z, J, \phi) : |r| \leq C, |z| \leq C_z, \frac{\pi}{N} < J < \frac{2\pi}{N}, \phi \in S^1 \right\}
\]

with \( C, C_z \) are fixed positive constants,

\[
\begin{align*}
\dot{r} &= Br + R(r_u, r_v, z, J, \phi; \sqrt{\varepsilon}) \\
\dot{z} &= Az + Z(r_u, r_v, z, J, \phi; \sqrt{\varepsilon}) \\
\dot{J} &= \sqrt{\varepsilon} E(r_u, r_v, z, J, \phi; \sqrt{\varepsilon}) \\
\dot{\phi} &= F_0(r_u, r_v, z, \phi) + \sqrt{\varepsilon} F(r_u, r_v, z, J, \phi; \sqrt{\varepsilon}) \quad (12)
\end{align*}
\]

where \( R, Z, E, F \) are nonlinear functions of class \( C^4 \), the matrix \( B \) is defined as \( B = \text{diag}(-a, a) \) where

\[
\pm a = \pm 2 \sqrt{(1 - \cos^2 \frac{2\pi}{N})} \omega^2 + h^{-2} (\omega^2 - N^2 \tan \frac{2\pi}{N})
\]

and the matrix \( A \) has purely imaginary eigenvalues \( \pm a_1, \ldots, a_2(M-1) \) and there exists a constant \( C_A \) such that

\[
|e^{A t} z| \leq C_A |z|.
\]

In the above local coordinates, the manifold \( \Pi \) satisfies the equations \( r_u = 0, r_v = 0, z = 0 \) and thus system (12) coincides with (10) and describes the dynamics on \( \Pi \). For \( \varepsilon = 0 \) the torus \( \mathcal{N}_c \) admits a unique codimension 2 center manifold

\[
\mathcal{M}_0 = \{(r_u, r_v, r_c) : r_u = h^{ca}(r_c; 0), \quad r_v = h^{ca}(r_c; 0), \quad r_c \in V \subset \mathbb{R}^{2M}\}
\]

where the functions \( h^{ca}, h^{cs} \) of class \( C^4 \) and \( r^c = (z, J, \phi) \). By the uniqueness of \( \mathcal{M}_0, \Pi \subset \mathcal{M}_0 \) holds implying \( h^{cs}(0, J, \phi) = 0, \quad h^{ca}(0, J, \phi) = 0 \). Then, there exists a unique, codimension 2 locally invariant manifold \( \mathcal{M}_c \) of class \( C^4 \) which depends on \( \varepsilon \)

\[
\mathcal{M}_c = \{r \in \mathcal{N} : r_u = h^{cs}(r_c; \varepsilon), \quad r_v = h^{ca}(r_c; \varepsilon), \quad r_c \in V \subset \mathbb{R}^{2M}\}
\]

and \( \Pi \subset \mathcal{M}_c \). The manifold \( \mathcal{M}_c \) admits codimension 1 local stable-unstable manifolds \( W_{loc}^{su}(\mathcal{M}_c) \) that are of class \( C^4 \) in \((r_u, r_v, r_c)\) and \( \varepsilon \), such that

\[
W_{loc}^{su}(\mathcal{M}_c) = \{r \in \mathcal{N} : r_u = h^s(r_u, r_v, r_c; \varepsilon), (r_u, r_v, r_c) \in \mathbb{R} \times \mathbb{R}^{2(M-1)} \times \mathbb{R} \times S^1\}
\]

\[
W_{loc}^{su}(\mathcal{M}_c) = \{r \in \mathcal{N} : r_u = h^u(r_u, r_v, r_c; \varepsilon), (r_u, r_v, r_c) \in \mathbb{R} \times \mathbb{R}^{2(M-1)} \times \mathbb{R} \times S^1\}
\]
The full Hamiltonian $H = H_0 + \varepsilon H_1$ restricts as

$$
\mathcal{H}_\varepsilon = H_{M_0} = H_0 + \varepsilon \mathcal{H} + \mathcal{O}(|z|^2, |z|, \varepsilon^{3/2})
$$

with the slow Hamiltonian $\mathcal{H}$ (near the resonance) defined in (11). From the system (12), we can write $\mathcal{H}_\varepsilon$ as

$$
\mathcal{H}_\varepsilon(z, J, \phi) = \varepsilon \mathcal{H}(J, \phi) + \frac{1}{2} \langle \mathcal{A} z, z \rangle + \mathcal{O}(|\varepsilon|^3, \sqrt{\varepsilon}|J| |z|^2, |z|, \varepsilon^{3/2})
$$

(13)

with $\mathcal{A} = \mathbb{J} \mathcal{A}$, here $\mathbb{J}$ is the symplectic matrix. As we mention above $\mathcal{H}$ generates a completely integrable flow on $\Pi$ with a family of invariant 1-tori (circles). The corresponding Hamiltonian equations can be derived from $\mathcal{H}_\varepsilon$ through the restricted symplectic form:

$$
\Omega_M = d\mathbb{f}(\omega + \sqrt{\varepsilon} J, \phi) \wedge d\mathbb{f}(\omega + \sqrt{\varepsilon} J, \phi) + dz_1 \wedge dz_2 + \sqrt{\varepsilon} d\phi \wedge dJ
$$

Since the matrix $\mathcal{A}$ has $2(M - 1)$ purely imaginary eigenvalues the first two terms in $\mathcal{H}_\varepsilon$, indicate the presence of $(2M - 1)$-dimensional tori on the slow manifold. However, the noncanonical structure of the symplectic form prevents us from using the Hamiltonian vector field on $\mathcal{M}_0$ in a near-integrable form to which existing versions of the KAM theorem can be applied (see Graff [1974]). The other difficulty is the presence of different time scales in the problem, which is due to the fact that we work close to a resonance, in a domain explicitly excluded by KAM-type methods. KAM tori can be constructed with "resonance islands" in the vicinity of the slow manifold $\Pi$.

3 Mel’nikov criteria and Homoclinic orbits

Our next goal is to develop criteria for the persistence of homoclinic solutions through the Hamiltonian structure of the system (1) with $\varepsilon \neq 0$. The perturbed AL-lattice can be put in the abstract form

$$
i\dot{q}_n = -\rho_n \left[ \frac{\partial H_0}{\partial q_n} + \varepsilon \frac{\partial H_1}{\partial q_n} \right]
$$

(14)

where

$$
H(q_n, a_1, a_2; \varepsilon) = H_0(q_n) + \varepsilon H_1(q_n, a_1, a_2)
$$

$$
H_0(q_n) = \frac{1}{\hbar^2} \sum_{n=1}^{N-1} \left\{ \tilde{q}_n(q_{n+1} + q_{n-1}) - \frac{2}{\hbar^2}(1 + \omega^2 \hbar^2)\ln \rho_n \right\}
$$

$$
H_1(q_n, a_1, a_2) = \frac{1}{\hbar^2} \sum_{n=1}^{N-1} \left\{ a_1(q_n + \tilde{q}_n) + a_2(q_n^2 + \tilde{q}_n^2) \right\} \ln \rho_n
$$

(15)

The evolution of any real-valued functional $S$ under the flow governed by eq. (14) for $\varepsilon = 0$, formally obeys:

$$
\frac{dS}{dt} = \{ S, H_0 \}
$$

where $\{ \cdot, \cdot \}$ the Poisson bracket on any two functional defined in eq. (3). The AL-lattice conserves the quantities

$$
I = \sum_{n=0}^{N-1} \ln(1 + \hbar^2 |q_n|^2), \quad F_1 = \frac{1}{D} \Delta(x^c; q)
$$
We consider real-valued functionals $\mathcal{S}$, which are smooth functions on $q_n$:

$$\mathcal{S}(q_n) = \sum_{n=0}^{N-1} s(q_n, \tilde{q}_n, q_{n+1}, \tilde{q}_{n+1}),$$

(16)

where $s$ is an analytic function of its arguments. The evolution of any such functional $\mathcal{S}$ that Poisson commutes with $H_0$ when evaluated along a solution of the perturbed AL-lattice (14), gives:

$$\frac{d\mathcal{S}}{dt} = \sum_{n=0}^{N-1} \left[ \frac{\partial \mathcal{S}}{\partial \tilde{q}_n} \frac{\partial s}{\partial q_n} + \frac{\partial \mathcal{S}}{\partial q_n} \frac{\partial s}{\partial \tilde{q}_n} \right] = \left\{ \mathcal{S}, H_0 \right\} - \varepsilon i \sum_{n=0}^{N-1} \left[ \frac{\partial \mathcal{S}}{\partial q_n} \frac{\partial H_1}{\partial \tilde{q}_n} - \frac{\partial \mathcal{S}}{\partial \tilde{q}_n} \frac{\partial H_1}{\partial q_n} \right] \rho_n$$

$$= -2\varepsilon \sum_{n=0}^{N-1} \text{Im} \left( \frac{\partial \mathcal{S}}{\partial q_n} \rho_n \frac{\partial H_1}{\partial q_n} \right)$$

then

$$\frac{d\mathcal{S}}{dt}(q_n) = -\varepsilon \Phi_{\mathcal{S}}(q_n(t))$$

(17)

where for any $q_n(t)$, the functional $\Phi_{\mathcal{S}}$ is defined by:

$$\Phi_{\mathcal{S}}(q_n(t)) = 2 \sum_{n=0}^{N-1} \text{Im} \left( \frac{\partial \mathcal{S}}{\partial q_n} \rho_n \frac{\partial H_1}{\partial q_n} \right)$$

(18)

We will consider here only those functional $\Phi_{\mathcal{S}}$ that satisfy

$$\left\{ \mathcal{S}, H_0 \right\} = \left\{ \mathcal{S}, I \right\} = \left\{ \mathcal{S}, F_1 \right\} = 0$$

(19)

Thus, it follows that $\Phi_{\mathcal{S}}$ is governed by the flows of $F_1, I$:

$$\left\{ \Phi_{\mathcal{S}}, F_1 \right\} = \left\{ \Phi_{\mathcal{S}}, I \right\} = 0$$

(20)

**Definition 3.1** A solution $Q_n(t)$ of AL-lattice which is homoclinic to a circle of equilibria $\mathcal{N}_\omega$ is said to persist under the Hamiltonian perturbation $H_1$ if and only if there exists an $\varepsilon$-dependent family of solutions $Q_n(t)$ of the perturbed problem that satisfies two requirements:

1. For each $\varepsilon$ it is homoclinic to the saddle point $\tilde{q}_c$ in the resonant annulus $\Lambda_\omega \subset \mathcal{N}_\omega$ in the sense

$$\lim_{|t| \to \infty} S(Q_n(t)) = S(\tilde{q}_c)$$

(21)

and

$$\lim_{t \to \pm \infty} \Phi_{\mathcal{S}}(Q_n(t)) = \Phi_{\mathcal{S}}(\tilde{q}_c) = 0$$

(22)

2. For any functional $\mathcal{S}$ that Poisson commutes with $H_0, I, F_1$ and

$$\lim_{\varepsilon \to 0} \Phi_{\mathcal{S}}(Q_n(t)) = \Phi_{\mathcal{S}}(Q_n(t))$$

(23)

**Eq. (17)** for the evolution of any conserved functional $\mathcal{S}$ evaluated at $Q_n(t)$ may be expressed as

$$\frac{d}{dt} \left( S(Q_n(t)) - S(\tilde{q}_c) \right) = -\varepsilon \Phi_{\mathcal{S}}(Q_n(t))$$

(24)

By eq. (21) the integration of eq. (24) gives

$$0 = -\frac{1}{\varepsilon} \left( S(Q_n(t)) - S(\tilde{q}_c) \right) \bigg|_{-\infty}^{+\infty} = \int_{-\infty}^{+\infty} \Phi_{\mathcal{S}}(Q_n(t)) dt$$

(25)

Taking the limit $\varepsilon \to 0$ in (25) we have the following:
Proposition 3.1 A necessary condition for the persistence of a AL-lattice solution $Q_n(t)$ that is homoclinic to a circle of equilibria $N_\omega$ is that it satisfy the Mel’nikov condition:

$$M_S(t_0) = \int_{-\infty}^{\infty} \Phi_S(Q_n(t)) \, dt = 0$$  (26)

For $S = I, F_1$, the above eq takes the form:

$$M_I(t_0) = 2 \int_{-\infty}^{\infty} \sum_{n=0}^{N-1} \text{Im} \left( \frac{\partial F_1}{\partial \varphi_n} \frac{\partial H_1}{\partial q_n} \right)(Q_n(t, t_0)) \, dt$$

$$M_{F_1}(t_0) = 2 \int_{-\infty}^{\infty} \sum_{n=0}^{N-1} \text{Im} \left( \frac{\partial F_1}{\partial \varphi_n} \frac{\partial H_1}{\partial q_n} \right)(Q_n(t, t_0)) \, dt$$

$$= a_1 k_1(\alpha, \gamma, \varphi, \omega, N) + a_2 k_2(\alpha, \gamma, \varphi, \omega, N)$$  (27)

with

$$\nabla F_1 = \left( \frac{\partial F_1}{\partial \varphi}, \frac{\partial F_1}{\partial q} \right), \quad \frac{\partial F_1}{\partial q} = a \exp[-i(\frac{\Delta \varphi}{2} + \varphi)] \Theta_1(Q_n, \varphi, \gamma, t)$$  (28)

where $\Theta_1$ is a known function of the general solutions of the Lax pair and $k_i$ are converging integrals.

Remark From the symplectic structure of our system, we can prove that the Mel’nikov function $M_I$ is identical zero.

Now, we are in a position to study the asymptotic behavior of the perturbed orbits near the center manifold $\mathcal{M}_c$ after the intersection of stable and unstable manifolds. We recall that in the new coordinates system $(r, z, J, \phi)$ the homoclinic orbits can be written as:

$$Q_n(t, t_0) = (r, z, J, \phi)(t - t_0)$$

(cf. eq. (8)). Application of the Mel’nikov formula in the resonant annulus $A_\omega$ for $S = H_0$ provides us with a sufficient condition for the persistence of homoclinic solution $Q_n(t)$, i.e the existence of orbits homoclinic to the periodic orbits inside the resonance.

Eq. (26) for $S = H_0$ becomes:

$$M_{H_0}(t_0) = \int_{-\infty}^{\infty} \left\{ (H_0, H_1) \right\}(Q_n(t, t_0)) \, dt = \int_{-\infty}^{\infty} \frac{d}{dt} H_1(Q_n(t, t_0)) \, dt$$

$$= H_1(Q_n(\gamma, \omega, N)) - H_1(Q_n(-\gamma, \omega, N))$$

$$= H_1(x_0, z_0, \omega + \sqrt{\omega} J) - H_1(x_0, z_0, \omega + \sqrt{\omega} J, \phi - \Delta \phi)$$  (29)

where we have used the new coordinates $(r, z, J, \phi)$ in the neighborhood of $\mathcal{M}_c$ and the asymptotic behavior of the homoclinic solutions $Q_n(t)$ as $t \rightarrow \pm \infty$, (cf. eq. (9)). For small $\varepsilon$ we Taylor-expand eq. (29) to obtain:

$$M_{H_0} = \mathcal{H}(J, \phi) - \mathcal{H}(J, \phi - \Delta \phi) + \mathcal{O}(\varepsilon$$

where $\mathcal{H}$ defined in eq.(11). A simple calculation gives:

$$M_{H_0} = 2W_\omega \left[ a_1 + 4\omega_2 \cos(\phi - \frac{\Delta \phi}{2}) \right] \sin\left( \frac{\Delta \phi}{2} \right) \sin\left( \phi - \frac{\Delta \phi}{2} \right)$$

Setting $M_{H_0} = 0$, it is easy to find the following solutions

$$\phi_1 = \frac{1}{2} \Delta \phi + \frac{\pi}{2}, \quad \phi_2 = \frac{1}{2} \Delta \phi + \frac{3\pi}{2}, \quad \phi_3 = \frac{1}{2} \Delta \phi + \cos^{-1}\left( -\frac{a_1}{4\omega_2} \right)$$
For \( \Delta \phi = 0, 2\pi \), we have
\[
D_\phi M_{H_0} \equiv (a_1 + 4\omega a_2 \cos \phi) \sin \phi = 0
\]
at \( \phi = 0, \pi, \cos^{-1}(-\frac{\omega}{\omega_1}) \). This means that \( D_\phi M_{H_0} \) is zero at the \( \phi \) values of the hyperbolic and elliptic fixed points in the resonance annulus.

For \( \Delta \phi \in [0, 2\pi] \) the perturbed solutions are asymptotic to the saddle points in the resonant area. Since all manifolds, as well as the Melnikov function depend differentiably on the parameters, there must be some value of \( M_{H_0} \) such that the trajectory corresponding to the zero of Melnikov function asymptotes to a trajectory in \( W^u(q_e) \cap A_\omega \) (where \( q_e \) is a saddle point), i.e. the boundary of the domain of attraction of elliptic points. Thus, we have the existence of an orbit homoclinic to the perturbed saddle point.

4 Hamiltonian Chaos and Numerical Simulations

When integrating numerically system (1) for \( \epsilon \neq 0 \), we generally expect to find chaotic solutions. In this section, we present numerical simulations that display this chaotic behavior in the neighborhood of the homoclinic orbits and for parameters which satisfy the Melnikov conditions, as explained in the previous section. At these parameter values, we use as diagnostics the Lyapunov exponents to check numerically for the presence of chaos.

We shall restrict ourselves to the case of system (1) with \( N = 4 \), displaying the phenomena of interest. This may appear as a simplification, but recently a so-called ‘homoclinic center–manifold’ theorem has been proved by Sandstede [1993, 1999]: Given a homoclinic orbit in an arbitrary (even infinite) dimensional system, there exists an invariant manifold along the homoclinic solution that is at least class \( C^1 \) and which contains all recurrent dynamics in a neighborhood of the homoclinic orbit. The dimension of this manifold depends on the linearization at the associated equilibrium point and the nature of the homoclinic trajectory itself. Roughly speaking, it is the dimension of the smallest possible phase space in which the particular homoclinic solution may generically arise.

For \( N = 4 \) we thus obtain from (1) a system of differential equations of the form:

\[
\begin{align*}
\dot{x} &= -i \left\{ 2 \frac{y - x}{h^2} + |x|^2 y - \omega^2 x \right\} + \epsilon f(x) \\
\dot{y} &= -i \left\{ \frac{z - 2y + x}{h^2} + |y|^2 (x + z) - 2\omega^2 y + \epsilon f(y) \right\} \\
\dot{z} &= -i \left\{ 2 \frac{y - z}{h^2} + |z|^2 y - \omega^2 z \right\} + \epsilon f(z)
\end{align*}
\]

(30)

with \( x = q_1, y = q_2, z = q_3 \), \( x, y, z \in \mathbb{C} \) and

\[
f(s) = a_1 (s^2 + |s|^2) + a_2 (s^2 + \bar{s}^2)s + (a_1 + 2a_2 \bar{s}) \left( \frac{1 + h^2 |s|^2}{h^2} \right) \ln(1 + h^2 |s|^2)
\]

In describing the chaotic behavior of system (30) we find it convenient to begin with simple solutions (fixed points and periodic orbits) in the neighborhood of the resonance annulus \( A_\omega \) for \( \omega = 4 \). As mentioned above, there are saddle and elliptic type fixed points in the invariant plane \( \Pi \) for \( \epsilon \)-small.
Figure 2: The chaotic dynamics of near-integrable Hamiltonian lattice (1) for $N = 4, \omega = 4.0, \varepsilon a_1 = 0.525, \varepsilon a_2 = 0.401$ in projections: (a) $(\text{Re}(x), \text{Im}(x))$ coordinates and (b) $(\text{Re}(x), \text{Re}(y), \text{Im}(z))$ coordinates.
In our computations the integration of the above system of ordinary differential equations is performed by the classical Runge–Kutta fourth order method, with initial conditions close to the resonance annulus $\Lambda_\omega$ of the reduced system and external parameters satisfying the Mel'nikov conditions. For small enough $\varepsilon > 0$, the chaotic dynamics of system (1) is not yet apparent and the orbits are seen to execute quasiperiodic behavior, as depicted in Fig. 2 for $\varepsilon a_1 = 0.525$, $\varepsilon a_2 = 0.401$, $\omega = 4.0$, $N = 4$. Observe, however, in Fig. 2(a) that the perfect regularity of the orbits displayed in Fig. 1 is not present. This difference is more vividly illustrated in the 3-D plots of Fig. 2(b).

Lyapunov exponents measure the degree of divergence of close trajectories in phase space in the course of time. They are a direct tool to infer the presence of chaos in the case where at least one Lyapunov exponent is larger than 0.

Given the dynamical system (1) in a $n = 2(M + 1)$-dimensional phase space (cf. Sec 1), we monitor the long-term evolution of an infinitesimal $n$-sphere of initial conditions, which becomes an $n$-ellipsoid due to the locally deforming nature of the flow. The Lyapunov exponents can either be estimated by making use of the equations, or else by using only a time series which has been generated by the system under scrutiny. We follow the first way, and apply the algorithms proposed in [Wolf et al., 1985].

To estimate the Lyapunov exponents with the help of the equations, the evolution of an infinitesimal 6-sphere is monitored in tangent space under the action of the linearized equations. This sphere turns into an ellipsoid, and we denote by $p_i$ the length of its $i$-th principal axis. Thus, the $i$-th Lyapunov exponent is defined in terms of the ellipsoidal principal axis $p_i$:

$$\lambda_i := \lim_{t \to \infty} \lambda_i(t) := \lim_{t \to \infty} \frac{1}{t} \log \frac{p_i(t)}{p_i(0)}$$

(31)

<table>
<thead>
<tr>
<th>$\varepsilon a_1$</th>
<th>0</th>
<th>0.525</th>
<th>0.8</th>
<th>0.95</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon a_2$</td>
<td>0</td>
<td>0.401</td>
<td>0.8</td>
<td>0.98</td>
<td>0.98</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\lambda_1$</th>
<th>0.0072</th>
<th>0.0074</th>
<th>0.0079</th>
<th>0.009</th>
<th>0.1276</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_2$</td>
<td>0.0048</td>
<td>0.0049</td>
<td>0.005</td>
<td>0.0069</td>
<td>0.0149</td>
</tr>
<tr>
<td>$\lambda_3$</td>
<td>0.0033</td>
<td>0.0038</td>
<td>0.0053</td>
<td>0.0059</td>
<td>0.0054</td>
</tr>
<tr>
<td>$\lambda_4$</td>
<td>-0.0032</td>
<td>-0.0035</td>
<td>-0.0049</td>
<td>-0.0057</td>
<td>-0.0054</td>
</tr>
<tr>
<td>$\lambda_5$</td>
<td>-0.0051</td>
<td>-0.0052</td>
<td>-0.0055</td>
<td>-0.0074</td>
<td>-0.0148</td>
</tr>
<tr>
<td>$\lambda_6$</td>
<td>-0.0072</td>
<td>-0.0075</td>
<td>-0.0077</td>
<td>-0.0088</td>
<td>-0.1278</td>
</tr>
</tbody>
</table>

| $d_A$ | 5.987 | 5.989 | 6.000 | 5.997 | 5.999 |

| $S_{\mu m}$ | -0.0002 | -0.0001 | 0.0001 | -0.0001 | -0.0001 |

Table 1: Lyapunov exponents for $N = 4$ and $\omega = 4.0$ and different sets of parameters $\varepsilon a_1$, $\varepsilon a_2$ for final time $\simeq 1000$ and initial condition $(\text{Re}(x), \text{Im}(x), \text{Re}(y), \text{Im}(y), \text{Re}(z), \text{Im}(z)) = (0.93, 1.558, 0.44, 0.6, 0.7, 0.8)$.

The signs of the Lyapunov exponents provide a qualitative picture of the dynamics since, if one of them is positive, this constitutes evidence for the presence of chaotic behavior. These exponents are
closely related also to the dimension \(d_\lambda\) of the associated chaotic dynamics through the equation

\[
d_\lambda = j + \frac{\sum_{i=1}^j \lambda_i}{|\lambda_{i+1}|}
\]

where \(j\) is the largest integer for which

\[
\sum_{i=1}^j \lambda_i \geq 0
\]

Let us now make some remarks concerning the accuracy of our computations: Observe that in the first column of Table 1, where \(\varepsilon = 0\) and our system of equations (40) is integrable, all Lyapunov exponents should be zero. Furthermore, in all cases, they should appear in positive-negative parts (due to the Hamiltonian structure of the equations) and hence should add up to zero. Note also that two of these exponents should be zero in the third and fourth row of Table 1 due to the constancy of the Hamiltonian. Finally, our accuracy is valid to the extent that the dimension of the dynamics in phase space is 6, as indicated by the value of \(d_\lambda\) in Table 1. Due to these remarks it is clear from Table 1 above that our results are accurate to order \(10^{-3}\), i.e. we can generally be sure of the first two digits. Clearly, for \(\varepsilon\) small enough, the chaotic behavior of the solutions is weak. The presence of large scale chaos is evident, however, for \(\varepsilon a_1 = 1.0\) and \(\varepsilon a_2 = 0.98\) where the positive exponents attain appreciably large values. Finally, when \(\varepsilon a_1 = \varepsilon a_2 = 1.0\) we find that the Lyapunov exponents steadily increase, until time \(t \approx 468\), when we have escape of the orbits to infinity. This is reminiscent of similar results found by [M. N. Vrahatis et al, 1997] for the orbits of a 4-dimensional symplectic map of accelerator dynamics.

5 Conclusions

Our motivation for this work was to investigate the chaotic dynamics of the Ablowitz–Ladik lattice with a Hamiltonian perturbation. In particular, we focused on the near-integrable Hamiltonian (1) and studied some homoclinic solutions of its unperturbed phase space which persist under the perturbation. Specifically, we have found that one can address this question studying families of special solutions of the lattice which are homoclinic in time to unstable plane wave solutions. We investigated these solutions through a Melnikov technique that utilizes the Hamiltonian structure of the lattice. It is worth mentioning, that the existence of conserved quantities, which Poisson commute with the functional \(\Phi_S\), is crucial to derive the Melnikov condition without using the geometric interpretation of the method. Moreover, the restriction of the perturbed problem to the center manifold is a 1-dof Hamiltonian system in order \(O(\sqrt{\varepsilon})\) and the linearized analysis gives the presence of saddle, center type fixed points.

We then integrated numerically the perturbed system for \(N = 4\) in the neighborhood of these homoclinic solutions and obtained the following: First, we verified the existence of chaos even for small values of the external parameters, by showing via Melnikov conditions that the stable and unstable manifolds of a circle of unstable equilibria intersect transversally. Secondly, using the differential equations of (1) we computed diagnostics such as Lyapunov exponents and verified that the system indeed has chaotic behavior near a fundamental resonance of the unperturbed system. This chaos, however, is transient, since for large enough perturbation our solutions eventually escape to infinity.

We also noted the noncanonical structure of the symplectic form and the presence of different time scales in our problem. These are main difficulties which prevent us from applying the existing versions of the KAM theory, [Graff, 1974]. KAM theory and diffusion phenomena in similar near-integrable Hamiltonian lattices are currently under study and results are expected to appear in a future publication.
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