Dynamics of PDE, Vol.3, No.3, 235-258, 2006

Arnold Diffusion of the Discrete Nonlinear Schrödinger Equation

Y. Charles Li

Communicated by Y. Charles Li, received April 3, 2006
and, in revised form, June 25, 2006.

ABSTRACT. In this article, we prove the existence of Arnold diffusion for an interesting specific system – discrete nonlinear Schrödinger equation. The proof is for the 5-dimensional case with or without resonance. In higher dimensions, the problem is open. Progresses are made by establishing a complete set of Melnikov-Arnold integrals in higher and infinite dimensions. The openness lies at the concrete computation of these Melnikov-Arnold integrals. New machineries introduced here into the topic of Arnold diffusion are the Darboux transformation and isospectral theory of integrable systems.

CONTENTS

1. Introduction

For a simple example posed by V. I. Arnold [**3**], the existence of the so-called Arnold diffusion has been proved (see e.g. [**3**] [**4**] [**14**]). The argument involves two parts: A calculation of the Melnikov-Arnold integrals [**3**] and a transversal intersection argument [**4**] supported by a λ-lemma [**14**]. Other arguments of variational type were also developed [**29**] [**31**] [**5**] [**7**].

Nevertheless, the theory of Arnold diffusion is far from complete [**13**] [**8**] [**28**] [**10**] [**30**] [**6**] [**9**] [**12**] [**15**] [**16**] [**11**]. The main challenge is dealing with high dimensional specific systems of interest in applications. When the dimensions of the

1991 *Mathematics Subject Classification.* 37, 34, 35, 78, 76.
Key words and phrases. Arnold diffusion, Darboux transformation, isospectral theory, Melnikov-Arnold integrals, λ-lemma, transition chain.

KAM tori are large, more Melnikov-Arnold integrals are needed to establish Arnold diffusion. Calculating these integrals is a dauting task if not impossible, even with computers. In an infinite dimensional phase space, even the dimensions of the KAM tori become a challenging issue. Are there infinite dimensional KAM tori ? in what form ? In the classical setting of a Banach space with angles-momenta coordinates, the challenge is how to deal with the perturbation v.s. the decay of the sequence of momenta. It is a very interesting problem.

The aim of the current article is to draw attention to two canonical systems of mathematical physics: The discrete nonlinear Schrödinger equation (DNLS) and its continuous version – the nonlinear Schrödinger equation (NLS). DNLS and NLS are integrable systems that describe many different phenomena in physics [**2**]. DNLS is an integrable finite difference discretization of NLS. An interesting fact about DNLS is that one can choose and change the dimensions of the phase space by selecting the number of particles in the discretization. For a two particle case, under periodic Hamiltonian perturbations, the resulting system is 5-dimensional, for which the existence of Arnold diffusion will be proved here. For a three particle case, the system is 7-dimensional, and will be a good testing ground for a higher dimensional theory.

The integrable theory offers the missing link from low dimension to high dimension via two powerful and beautiful machineries: Darboux transformation and isospectral theory. Darboux transformation generates explicit expressions of separatrices, while isospectral theory produces all the Melnikov vectors. Together they provide a complete set of Melnikov-Arnold integrals with elegant universal formulae. This is the case for both DNLS and NLS [**17**] [**18**] [**19**] [**20**] [**21**]. On the other hand, specific calculation of these integrals is the challenge. For the purpose of proving the existence of chaos, often one Melnikov integral is enough and easily computable [**19**] [**21**] [**22**] [**25**] [**26**]. The reason is that one can utilize locally invariant center manifolds instead of KAM tori. For the purpose of Arnold diffusion, local invariance (i.e. orbits can only enter or leave the submanifold through its boundaries) is not enough. This is due to the second part of the argument for Arnold diffusion mentioned above. To establish a λ-lemma, one needs the tori to be invariant (not locally invariant). For a different application of λ-lemma in (1). establishing shadowing lemma in infinite dimensional autonomous systems, (2). proving the existence of homoclinic tubes and heteroclinically tubular cycles, (3). proving the existence of tubular chaos, (4). proving the existence of chaos cascade; we refer the readers to [**23**] [**24**] [**25**] [**26**].

The article is organized as follows: Section 2 deals with isospectral theory and Darboux transformation for both DNLS and NLS. Section 3 deals with Arnold diffusion for a 5-dimensional perturbed DNLS.

2. Isospectral Theory and Darboux Transformation

In this section, we are going to present the isospectral theory and Darboux transformation for both the discrete nonlinear Schrödinger equation (DNLS) and the nonlinear Schrödinger equation (NLS).

2.1. Discrete Nonlinear Schrödinger Equation. Consider the discrete nonlinear Schrödinger equation (DNLS),

$$i\dot{q}_n = \frac{1}{h^2}[q_{n+1} - 2q_n + q_{n-1}] + |q_n|^2(q_{n+1} + q_{n-1}) - 2\omega^2 q_n \ , \tag{2.1}$$

where q_n's are complex-valued, $i = \sqrt{-1}$ is the imaginary unit, ω is a positive parameter, and q_n satisfies the periodic boundary condition and even constraint,

$$q_{n+N} = q_n, \quad q_{-n} = q_n \ , \tag{2.2}$$

where N is a positive integer $N \geq 3$ and $h = 1/N$. The DNLS (2.1) is a $2(M+1)$-dimensional system, where $M = N/2$ (N even) and $M = (N-1)/2$ (N odd). The DNLS can be rewritten in the Hamiltonian form

$$i\dot{q}_n = \rho_n \partial H_0 / \partial \overline{q_n} \ , \tag{2.3}$$

where $\rho_n = 1 + h^2 |q_n|^2$ and

$$H_0 = \frac{1}{h^2} \sum_{n=0}^{N-1} \left\{ \overline{q_n}(q_{n+1} + q_{n-1}) - \frac{2}{h^2}(1 + \omega^2 h^2) \ln \rho_n \right\} .$$

The phase space is defined as

$$\mathcal{S} = \left\{ \vec{q} = (\mathbf{q}, \bar{\mathbf{q}}) \middle| \ \mathbf{q} = (q_0, q_1, ..., q_{N-1}), \ q_{N-n} = q_n \ (1 \leq n \leq N-1) \right\} .$$

In $\mathcal{S}$ (viewed as a vector space over the real numbers), we define the inner product, for any two points $\vec{q}^{\,+}$ and $\vec{q}^{\,-}$, as follows:

$$\langle \vec{q}^{\,+}, \vec{q}^{\,-} \rangle = \sum_{n=0}^{N-1} (q_n^+ \overline{q_n^-} + \overline{q_n^+} q_n^-) \ .$$

And the norm of $\vec{q}$ is defined as $\|\vec{q}\,\|^2 = \langle \vec{q}, \vec{q} \rangle$.

Remark 2.1. In the expression of H_0, both $\sum_{n=0}^{N-1} [\overline{q_n}(q_{n+1} + q_{n-1})]$ and $I = \frac{1}{h^2} \sum_{n=0}^{N-1} \ln \rho_n$ are constants of motion too. I will be used later to establish Arnold diffusion in the non-resonant case. Also the constant of motion D given by $D^2 = \prod_{n=0}^{N-1} \rho_n$ will play an important role in the isospectral theory. In the continuum limit (i.e. $h \to 0$), the Hamiltonian H_0 has a limit in the manner: $hH_0 \to H_c$, where H_c is the Hamiltonian for NLS, $H_c = -\int_0^1 [|q_x|^2 + 2\omega^2 |q|^2 - |q|^4] dx$. Also as $h \to 0$, $D \to 1$.

2.2. Isospectral Theory of DNLS. For more details on the topic of this subsection, see [**18**]. DNLS has the Lax pair [**1**]

$$\varphi_{n+1} = L_n \varphi_n, \tag{2.4}$$

$$\dot{\varphi}_n = B_n \varphi_n, \tag{2.5}$$

where

$$L_n = \begin{pmatrix} z & ihq_n \\ ih\overline{q_n} & 1/z \end{pmatrix},$$

$$B_n = \frac{i}{h^2} \begin{pmatrix} 1 - z^2 + 2i\lambda h - h^2 q_n \overline{q_{n-1}} + \omega^2 h^2 & -izhq_n + (1/z) ihq_{n-1} \\ -izh\overline{q_{n-1}} + (1/z) ih\overline{q_n} & \frac{1}{z^2} - 1 + 2i\lambda h + h^2 \overline{q_n} q_{n-1} - \omega^2 h^2 \end{pmatrix},$$

and where $z = \exp(i\lambda h)$. Compatibility of the over determined system (2.4,2.5) gives the "Lax representation"

$$\dot{L}_n = B_{n+1} L_n - L_n B_n$$

of the DNLS (2.1). Focusing our attention upon the discrete spatial part (2.4) of the Lax pair, let $M_n = M_n(z, \vec{q})$ be the 2×2 fundamental matrix solution such that M_0 is the 2×2 identity matrix. The *Floquet discriminant* $\Delta : \mathbb{C} \times \mathcal{S} \to \mathbb{C}$ is defined by

$$\Delta = \frac{1}{D} \text{ trace } M_N(z, \vec{q}) \ ,$$

where $D^2 = \prod_{n=0}^{N-1} \rho_n$. The isospectral theory starts from the fact that for any $z \in \mathbb{C}$, $\Delta(z, \vec{q})$ is a constant of motion of DNLS. An easy way to understand this is that as q_n evolves in time according to DNLS, the parameter z in the Lax pair does not change. $\Delta(z, \vec{q})$ is a meromorphic function in z of degree $(+N, -N)$, and provides $(M+1)$ functionally independent constants of motion, where $M = N/2$ (N even), $M = (N-1)/2$ (N odd). There are many ways to generate $(M+1)$ functionally independent constants of motion from Δ. The approach which proved to be most convenient is by employing all the critical points z^c of $\Delta(z, \vec{q})$:

$$\frac{\partial \Delta}{\partial z}(z^c, \vec{q}) = 0 \ .$$

DEFINITION 2.2. We define a sequence of $(M+1)$ constants of motion F_j as follows

$$F_j(\vec{q}) = \Delta(z_j^c(\vec{q}), \vec{q}) \ , \quad (j = 1, \cdots, M+1) \ . \tag{2.6}$$

There is a good description on the locations of these critical points z_j^c in the NLS setting [**19**]. These F_j's can be used to build a complete set of Melnikov-Arnold integrals for the Arnold diffusion purpose. The Melnikov vectors are given by the gradients of these F_j's.

THEOREM 2.3. *Let $z_j^c(\vec{q})$ be a simple critical point, then*

$$\begin{pmatrix} \frac{\partial F_j}{\partial q_n} \\ \\ \frac{\partial F_j}{\partial \overline{q_n}} \end{pmatrix} = \frac{ih(\zeta - \zeta^{-1})}{2W_{n+1}} \begin{pmatrix} \psi_{n+1}^{(+,2)}\psi_n^{(-,2)} + \psi_n^{(+,2)}\psi_{n+1}^{(-,2)} \\ \\ -\psi_{n+1}^{(+,1)}\psi_n^{(-,1)} - \psi_n^{(+,1)}\psi_{n+1}^{(-,1)} \end{pmatrix} , \tag{2.7}$$

where $\psi_n^{\pm} = (\psi_n^{(\pm,1)}, \psi_n^{(\pm,2)})^T$, (T: transpose), are two Bloch solutions of the Lax pair (2.4,2.5) at $(z_j^c, \vec{q})$ such that

$$\psi_n^{\pm} = D^{n/N}\zeta^{\pm n/N}\tilde{\psi}_n^{\pm} \ ,$$

where $\tilde{\psi}_n^{\pm}$ are periodic in n with period N, ζ is a complex constant, and $W_n =$ det (ψ_n^+, ψ_n^-) is the Wronskian.

For a perturbation $H_0 + \epsilon H_1$ of the Hamiltonian H_0, a complete set of Melnikov-Arnold integrals is then given by

$$I_j = \int_{-\infty}^{\infty} \sum_{n=0}^{N-1} 2 \text{ Im} \left[\frac{\partial F_j}{\partial q_n} \rho_n \frac{\partial H_1}{\partial \overline{q_n}} \right] dt \ , \quad (j = 1, \cdots, M+1) \ ,$$

which are evaluated on the unstable manifolds of tori that persist into KAM tori, where $\frac{\partial F_j}{\partial q_n}$ is given by (2.7). Expression (2.7) is a universal expression for all the Melnikov vectors. The challenge is of course how to compute these I_j's. The difficulty lies at how to obtain expressions of the orbit q_n and the corresponding $\psi_n^{\pm}$. By utilizing Darboux transformations, these expressions can be obtained even by hand in some cases.

2.3. Darboux Transformation of DNLS. For more details on the topic of this subsection, see [**18**]. Expressions of unstable manifolds of tori can be generated via Darboux transformations. For DNLS, such a Darboux transformation was established in [**17**].

Let q_n be any solution of DNLS. Pick $z = z^d$ ($|z^d| \neq 1$) at which the linear operator L_n in the Lax pair (2.4)-(2.5) has two linearly independent periodic solutions (or anti-periodic solutions) $\phi_n^\pm$ in the sense:

$$\phi_{n+N}^\pm = D\phi_n^\pm \ , \quad (\text{or } \phi_{n+N}^\pm = -D\phi_n^\pm) \ ,$$

where D is defined above. Let

$$\phi_n = (\phi_{n1}, \phi_{n2})^T = c^+\phi_n^+ + c^-\phi_n^- \ ,$$

where c^+ and c^- are complex parameters. Define the matrix Γ_n by

$$\Gamma_n = \begin{pmatrix} z + (1/z)a_n & b_n \\ c_n & -1/z + zd_n \end{pmatrix},$$

where

$$\begin{aligned} a_n &= \frac{z^d}{\overline{z^d}^2 \Delta_n}\Big[|\phi_{n2}|^2 + |z^d|^2|\phi_{n1}|^2\Big], \\ d_n &= -\frac{1}{z^d \Delta_n}\Big[|\phi_{n2}|^2 + |z^d|^2|\phi_{n1}|^2\Big], \\ b_n &= \frac{|z^d|^4 - 1}{\overline{z^d}^2 \Delta_n}\phi_{n1}\overline{\phi_{n2}}, \\ c_n &= \frac{|z^d|^4 - 1}{|z^d|^2 \Delta_n}\overline{\phi_{n1}}\phi_{n2}, \\ \Delta_n &= -\frac{1}{\overline{z^d}}\Big[|\phi_{n1}|^2 + |z^d|^2|\phi_{n2}|^2\Big]. \end{aligned}$$

From these formulae, we see that

$$\overline{a_n} = -d_n, \quad \overline{b_n} = c_n.$$

THEOREM 2.4 (Darboux Transformation [**17**]). *Define* Q_n *and* Ψ_n *by*

$$Q_n = \frac{i}{h} b_{n+1} - a_{n+1} q_n \ , \quad \Psi_n = \Gamma_n \psi_n \ ,$$

where ψ_n *solves the Lax pair (2.4)-(2.5) at* (q_n, z). *Then* Q_n *is also a solution of DNLS, and* Ψ_n *solves the Lax pair (2.4)-(2.5) at* (Q_n, z).

In principle, by choosing q_n to be orbits on the tori, one can generate Q_n to be orbits on the unstable manifolds of the tori. In special cases, Q_n can be calculated by hands.

Next we present an example. Define the 2-dimensional invariant plane

$$\Pi = \{\vec{q} \in \mathcal{S} \mid q_n = q \ , \quad \forall n\} \ . \tag{2.8}$$

On Π, the solutions of DNLS are given by the periodic orbits (1-tori)

$$q_n = q_c \ , \ \forall n; \quad q_c = a \exp\left\{-i[2(a^2 - \omega^2)t - \gamma]\right\} \ , \tag{2.9}$$

where a and γ are real constants. We choose the amplitude a in the following range so that the unstable direction of q_c is 1-dimensional

$$N \tan \frac{\pi}{N} < a < N \tan \frac{2\pi}{N} , \quad \text{when } N > 3 ,$$

(2.10)

$$3 \tan \frac{\pi}{3} < a < \infty , \quad \text{when } N = 3 .$$

Increasing the unstable dimensions of q_c amounts to iterations of the Darboux transformation which are still doable by hands, and does not add difficulty substantially in the Arnold diffusion problem. To apply the Darboux transformation we choose

$$z^d = \sqrt{\rho} \cos \frac{\pi}{N} + \sqrt{\rho \cos^2 \frac{\pi}{N} - 1} ,$$

where $\rho = 1 + h^2 a^2$. This z^d is also a critical point of Δ. We label it by $z_1^c = z^d$. Direct calculation leads to the following formulae

$$Q_n = q_c \left[\Gamma / \Lambda_n - 1 \right] , \tag{2.11}$$

$$\left(\begin{array}{c} \frac{\partial F_1}{\partial q_n} \\ \\ \frac{\partial F_1}{\partial \overline{q_n}} \end{array} \right) \Bigg|_{Q_n} = K [K_n]^{-1} \operatorname{sech}[2\mu t + 2p] \left(\begin{array}{c} X_n^1 \\ X_n^2 \end{array} \right) , \tag{2.12}$$

where

$$\begin{aligned}
\Gamma &= 1 - \cos 2\varphi - i \sin 2\varphi \tanh[2\mu t + 2p] , \\
\Lambda_n &= 1 \pm \cos \varphi [\cos \beta]^{-1} \operatorname{sech}[2\mu t + 2p] \cos[2n\beta] , \\
K &= -2N(1 - \hat{z}^4)[8a\rho^{3/2}\hat{z}^2]^{-1} \sqrt{\rho \cos^2 \beta - 1} , \\
K_n &= \Big[\cos \beta \pm \cos \varphi \operatorname{sech}[2\mu t + 2p] \cos[2(n-1)\beta] \Big] \times \\
&\quad \Big[\cos \beta \pm \cos \varphi \operatorname{sech}[2\mu t + 2p] \cos[2(n+1)\beta] \Big] , \\
X_n^1 &= \Big[\cos \beta \operatorname{sech} [2\mu t + 2p] \pm (\cos \varphi \\
&\quad - i \sin \varphi \tanh[2\mu t + 2p]) \cos[2n\beta] \Big] e^{i2\theta(t)} , \\
X_n^2 &= \Big[\cos \beta \operatorname{sech} [2\mu t + 2p] \pm (\cos \varphi \\
&\quad + i \sin \varphi \tanh[2\mu t + 2p]) \cos[2n\beta] \Big] e^{-i2\theta(t)} , \\
&\quad \beta = \pi/N , \quad \mu = 2h^{-2} \sqrt{\rho} \sin \beta \sqrt{\rho \cos^2 \beta - 1} , \\
&\quad \rho = 1 + h^2 a^2 , \quad h = 1/N, \quad \hat{z} = \sqrt{\rho} \cos \beta + \sqrt{\rho \cos^2 \beta - 1} , \\
&\quad \theta(t) = (a^2 - \omega^2)t - \gamma/2 , \quad hae^{i\varphi} = \sqrt{\rho \cos^2 \beta - 1} + i \sqrt{\rho} \sin \beta .
\end{aligned}$$

and p is a real parameter. One can easily see that Q_n represents homoclinic orbits asymptotic to the periodic orbits q_c: As $t \to \pm\infty$,

$$Q_n \to q_c e^{i(\pi \pm 2\varphi)} .$$

The union

$$\bigcup_{\gamma\in[0,2\pi]} Q_n$$

represents the 2-dimensional unstable (=stable) manifold of the 1-torus (2.9). When $N > 3$, the 1-torus also has a center manifold of codimension 2.

2.4. Nonlinear Schrödinger Equation. Consider the nonlinear Schrödinger equation (NLS),

$$iq_t = q_{xx} + 2[|q|^2 - \omega^2]q \ , \tag{2.13}$$

where $q = q(t,x)$ is a complex-valued function of the two real variables t and x, t represents time, and x represents space. $q(t,x)$ is subject to periodic boundary condition of period 2π, and even constraint, i.e.

$$q(t, x + 2\pi) = q(t, x) \ , \quad q(t, -x) = q(t, x) \ .$$

ω is a positive parameter. The DNLS (2.1) is an integrable finite difference discretization of the NLS. The NLS can be rewritten in the Hamiltonian form

$$i\dot{q} = \partial H_0 / \partial \bar{q} \ , \tag{2.14}$$

where

$$H_0 = -\int_0^{2\pi} \left[|q_x|^2 + 2\omega^2|q|^2 - |q|^4\right] dx \ .$$

The phase space is defined as

$$\mathcal{S} = \left\{ \vec{q} = (q, \bar{q}) \middle| \ q \in H^k \ , \quad (k \geq 1) \right\} ,$$

where H^k is the Sobolev space of periodic and even functions.

2.5. Isospectral Theory of NLS. For more details on the topic of this subsection, see [**19**]. NLS has the Lax pair

$$\psi_x = U\psi \ , \tag{2.15}$$

$$\psi_t = V\psi \ , \tag{2.16}$$

where

$$U = i \begin{pmatrix} \lambda & q \\ \bar{q} & -\lambda \end{pmatrix} ,$$

$$V = i \begin{pmatrix} 2\lambda^2 - |q|^2 + \omega^2 & 2\lambda q - iq_x \\ 2\lambda\bar{q} + i\overline{q_x} & -2\lambda^2 + |q|^2 - \omega^2 \end{pmatrix} .$$

Focusing our attention on the spatial part (2.15) of the Lax pair (2.15,2.16), we can define the fundamental matrix solution $M(x)$ such that $M(0)$ is the 2×2 identity matrix. Then the *Floquet discriminant* Δ is defined as

$$\Delta = \text{ trace } M(2\pi) \ .$$

The isospectral theory starts from the fact that for any $\lambda \in \mathbb{C}$, $\Delta(\lambda, \vec{q})$ is a constant of motion of NLS. $\Delta = \Delta(\lambda, q)$ is an entire function in both λ and $\vec{q}$. Δ provides enough functionally independent constants of motion to make the NLS (2.13) integrable in the classical Liouville sense. There are many ways to generate these functionally independent constants of motion from Δ. The approach which proved to be most convenient is by employing all the critical points λ^c of $\Delta(\lambda, \vec{q})$:

$$\frac{\partial \Delta}{\partial \lambda}(\lambda^c, \vec{q}) = 0 \ .$$

For each $\vec{q}$, there is a sequence of critical points $\{\lambda_j^c\}$ whose locations can be estimated [**19**].

DEFINITION 2.5. We define a sequence of constants of motion F_j as follows

$$F_j(\vec{q}) = \Delta(\lambda_j^c(\vec{q}), \vec{q}) \ .$$

These F_j's can be used to build a complete set of Melnikov-Arnold integrals for the Arnold diffusion purpose. The Melnikov vectors are given by the gradients of these F_j's.

THEOREM 2.6. *Let $\lambda_j^c(\vec{q})$ be a simple critical point, then*

$$\begin{pmatrix} \frac{\partial F_j}{\partial q} \\ \\ \frac{\partial F_j}{\partial \overline{q}} \end{pmatrix} = i \frac{\sqrt{\Delta^2 - 4}}{W(\psi^+, \psi^-)} \begin{pmatrix} \psi_2^+ \psi_2^- \\ -\psi_1^+ \psi_1^- \end{pmatrix} \ , \tag{2.17}$$

where $\psi^{\pm} = (\psi_1^{\pm}, \psi_2^{\pm})^T$, ($T$: transpose), are two Bloch solutions of the Lax pair (2.15)-(2.16) at $(\lambda_j^c, \vec{q})$ such that

$$\psi^{\pm}(x) = e^{\pm \sigma x} \tilde{\psi}^{\pm}(x) \ ,$$

where σ is a complex constant and $\tilde{\psi}^{\pm}(x)$ are periodic in x with period 2π,

$$W(\psi^+, \psi^-) = \psi_1^+ \psi_2^- - \psi_2^+ \psi_1^-$$

is the Wronskian, and Δ is evaluated at $\lambda = \lambda_j^c$.

For a perturbation $H_0 + \epsilon H_1$ of the Hamiltonian H_0, a complete set of Melnikov-Arnold integrals is then given by

$$I_j = \int_{-\infty}^{\infty} \int_0^{2\pi} 2 \ \text{Im} \left[\frac{\partial F_j}{\partial q} \frac{\partial H_1}{\partial \overline{q}} \right] dx dt \ ,$$

which are evaluated on the unstable manifolds of tori that persist into KAM tori, where $\frac{\partial F_j}{\partial q}$ is given by (2.17). Expression (2.17) is a universal expression for all the Melnikov vectors. The challenge is of course how to compute these I_j's. The difficulty lies at how to obtain expressions of the orbit q and the corresponding $\psi^{\pm}$. By utilizing Darboux transformations, these expressions can be obtained even by hand in some cases. Also as mentioned in the introduction, there is the issue of elusiveness of infinite dimensional KAM tori. As $j \to \infty$, The magnitude of I_j v.s. the size of the perturbation ϵ is another tricky problem.

2.6. Darboux Transformation of NLS. For more details on the topic of this subsection, see [**19**]. Expressions of unstable manifolds of tori can be generated via Darboux transformations. For NLS, such a Darboux transformation was also known.

Let q be any solution of NLS. Pick $\lambda = \nu$ (complex constant) at which (2.15) has two linearly independent periodic solutions (or anti-periodic solutions) $\phi^{\pm}$ in the sense:

$$\phi^{\pm}(x + 2\pi) = \phi^{\pm}(x) \ , \quad (\text{or } \phi^{\pm}(x + 2\pi) = -\phi^{\pm}(x)) \ .$$

Let

$$\phi = c_+\phi^+ + c_-\phi^- \ ,$$

where c_+ and c_- are complex parameters. Define the matrix G by

$$G = \Gamma \begin{pmatrix} \lambda - \nu & 0 \\ 0 & \lambda - \bar{\nu} \end{pmatrix} \Gamma^{-1} \ ,$$

where

$$\Gamma = \begin{pmatrix} \phi_1 & -\overline{\phi_2} \\ \phi_2 & \overline{\phi_1} \end{pmatrix} \ .$$

THEOREM 2.7 (Darboux Transformation). *Define Q and Ψ by*

$$Q = q + 2(\nu - \bar{\nu}) \frac{\phi_1 \overline{\phi_2}}{|\phi_1|^2 + |\phi_2|^2} \ , \quad \Psi = G\psi \ ,$$

where ψ solves the Lax pair (2.15)-(2.16) at (q, λ). Then Q is also a solution of NLS, and Ψ solves the Lax pair (2.15)-(2.16) at (Q, λ).

In principle, by choosing q to be orbits on the tori, one can generate Q to be orbits on the unstable manifolds of the tori. In special cases, Q can be calculated by hands.

Next we present an example. Define the 2-dimensional invariant plane

$$\Pi = \{\vec{q} \in \mathcal{S} \mid \partial_x q = 0\} \ .$$

On Π, the solutions of NLS are given by the same periodic orbits (1-tori) as in (2.9)

$$q_c = a \exp\left\{-i[2(a^2 - \omega^2)t - \gamma]\right\} \ , \tag{2.18}$$

where a and γ are real constants. We choose the amplitude a in the range $a \in (1/2, 1)$ so that the unstable direction of q_c is 1-dimensional. Increasing the unstable dimensions of q_c amounts to iterations of the Darboux transformation which are still doable by hands [**21**], and does not add difficulty substantially in the Arnold diffusion problem. To apply the Darboux transformation we choose

$$\nu = i\sigma \ , \quad \sigma = \sqrt{a^2 - 1/4} \ .$$

This ν is also a critical point of Δ. We label it by $z_1^c = \nu$. Direct calculation leads to

$$\begin{aligned} Q &= q_c \left[1 \pm \sin\vartheta_0 \ \mathrm{sech}\tau \cos x\right]^{-1} \\ &\quad \cdot \left[\cos 2\vartheta_0 - i \sin 2\vartheta_0 \tanh\tau \mp \sin\vartheta_0 \ \mathrm{sech}\tau \cos x\right] \ , \\ \begin{pmatrix} \frac{\partial F_1}{\partial q} \\ \frac{\partial F_1}{\partial \bar{q}} \end{pmatrix} \Bigg|_Q &= \frac{1}{4} a^{-2} i(\nu - \bar{\nu}) \sqrt{\Delta(\nu)\Delta''(\nu)} \frac{1}{(|u_1|^2 + |u_2|^2)^2} \begin{pmatrix} \overline{q_c} \ \overline{u_1}^{\ 2} \\ -q_c \ \overline{u_2}^{\ 2} \end{pmatrix} \ , \end{aligned}$$

where

$$\begin{aligned} u_1 &= \cosh\frac{\tau}{2} \cos z - i \sinh\frac{\tau}{2} \sin z \ , \\ u_2 &= -\sinh\frac{\tau}{2} \cos(z - \vartheta_0) + i \cosh\frac{\tau}{2} \sin(z - \vartheta_0) \ , \\ & a e^{i\vartheta_0} = \frac{1}{2} + \nu \ , \quad \tau = 2\sigma t - \rho \ , \quad z = x/2 + \vartheta_0/2 \mp \pi/4 \ , \end{aligned}$$

and ρ is a real parameter. As $t \to \pm\infty$,

$$Q \to q_c e^{\mp i2\vartheta_0} \ .$$

The union

$$\bigcup_{\gamma\in[0,2\pi]} Q$$

represents the 2-dimensional unstable (=stable) manifold of the 1-torus (2.18). The 1-torus also has a center manifold of codimension 2.

3. Arnold Diffusion

To establish the existence of Arnold diffusion, one needs three ingredients: (1). Melnikov-Arnold integrals, (2). A λ-lemma, (3). A transversal intersection argument. Melnikov-Arnold integrals have been studied above. Next we discuss the other two ingredients.

LEMMA 3.1 (The λ-lemma of Fontich-Martin [**14**]). *Let F be a C^2 diffeomorphism in $\mathbb{R}^n$, $\mathbb{T}$ be a C^2 invariant torus in $\mathbb{R}^n$. The dynamics on $\mathbb{T}$ is quasi-periodic. $\mathbb{T}$ has C^2 unstable, stable and center manifolds (W^u, W^s, W^c). Let Γ be a C^1 manifold intersecting transversally W^s at a point. Then*

$$W^u \subset \overline{\bigcup_{m\geq 0} F^m(\Gamma)} \ .$$

REMARK 3.2. Like every other λ-lemma, the claim is very intuitive, but the proof is always delicate. The proof in [**14**] takes about eight pages. For a quick glance of the basic idea, see e.g. [**23**]. It turns out to be crucial to use Fenichel's fiber coordinates. With respect to base points, Fenichel fibers drop one degree of smoothness. That is why C^2 smoothness is required in the lemma to obtain C^1 families of C^2 unstable and stable Fenichel fibers. Using the Fenichel's fiber coordinates, W^u and W^s are rectified, i.e. they coincide with their tangent bundles. This makes the estimate a lot easier. Fenichel fibers also make it easier to track orbits inside W^u and W^s via the fiber base points in $\mathbb{T}$. The main argument is to track the tangent space of a submanifold S of Γ starting from the intersection point of Γ and W^s. After enough iterations of F, one can obtain some estimate of closeness to W^u. The novelty of [**14**] is that they also track the tangent space at every point in S and off W^s. This is necessary in order to obtain the claim of the lemma. The claim is proved by showing that any neighborhood of any point on W^u has a nonempty intersection with $F^m(S)$ for some m. The claim of the lemma should also be true in proper infinite dimensional settings.

DEFINITION 3.3 (Transition Chain). A finite or infinite sequence of tori $\{\mathbb{T}_j\}$ forms a transition chain if $W^s(\mathbb{T}_j)$ intersects transversally $W^u(\mathbb{T}_{j+1})$ at some point, for all j, and dynamics on $\mathbb{T}_j$ is quasi-periodic.

LEMMA 3.4 (Arnold [**4**]). *Let $\{\mathbb{T}_j\}$ ($1 \leq j \leq N$) be a finite transition chain. Then an arbitrary neighborhood of an arbitrary point in $W^u(\mathbb{T}_1)$ is connected to an arbitrary neighborhood of an arbitrary point in $W^s(\mathbb{T}_N)$ by an orbit.*

PROOF. Let Ω_1 be an arbitrary neighborhood of an arbitrary point $u_1 \in W^u(\mathbb{T}_1)$. Let $\bar{B}_{u_1}(r_1) \subset \Omega_1$ be a closed ball of radius $r_1 > 0$ centered at u_1. Then using the λ-lemma 3.1, one can find

$$\bar{B}_{u_N}(r_N) \subset \bar{B}_{u_{N-1}}(r_{N-1}) \cdots \subset \bar{B}_{u_2}(r_2) \subset \bar{B}_{u_1}(r_1) \tag{3.1}$$

such that

$$u_j \in W^u(\mathbb{T}_j)\ , \quad r_j > 0\ , \quad (1 \le j \le N)\ .$$

Indeed, by the λ-lemma 3.1,

$$B_{u_1}(r_1) \cap W^u(\mathbb{T}_2) \neq \emptyset$$

where $B_{u_1}(r_1)$ is the open ball. Then one can find

$$u_2 \in B_{u_1}(r_1) \cap W^u(\mathbb{T}_2)\ , \text{ and } \bar{B}_{u_2}(r_2) \subset B_{u_1}(r_1)\ .$$

Again by the λ-lemma 3.1,

$$B_{u_2}(r_2) \cap W^u(\mathbb{T}_3) \neq \emptyset\ ,$$

and one can find

$$u_3 \in B_{u_2}(r_2) \cap W^u(\mathbb{T}_3)\ , \text{ and } \bar{B}_{u_3}(r_3) \subset B_{u_2}(r_2)\ ,$$

and so on. Let Ω_N be an arbitrary neighborhood of an arbitrary point in $W^s(\mathbb{T}_N)$. Inside Ω_N, one can find a C^1 submanifold intersecting transversally $W^s(\mathbb{T}_N)$ at the point. Again by the λ-lemma 3.1,

$$B_{u_N}(r_N) \cap F^m(\Omega_N) \neq \emptyset \text{ for some } m\ .$$

Thus Ω_1 and Ω_N are connected by an orbit. □

REMARK 3.5. It is easy to see that around the connecting orbit, there is in fact a connecting flow tube [**27**] [**24**] [**25**] [**26**]

$$\bigcup_{0 \le m \le M} F^m(D) \quad \text{for some } M$$

where D is a neighborhood. When $N = \infty$, relation (3.1) leads to a point in the intersection

$$u \in \bigcap_{j=0}^{\infty} \bar{B}_{u_j}(r_j)\ .$$

Starting from u, one obtains a connecting orbit. In a Banach space setting, if $N = \infty$, then one can choose $r_{j+1} \le \frac{1}{2} r_j$ for any j in (3.1). Choosing an arbitrary point v_j in $\bar{B}_{u_j}(r_j)$, one gets a Cauchy sequence $\{v_j\}$. Thus

$$\lim_{j \to \infty} v_j = v \in \bigcap_{j=0}^{\infty} \bar{B}_{u_j}(r_j)\ .$$

Starting from v, one still obtains a connecting orbit.

3.1. Arnold Diffusion of DNLS ($N = 3$, Non-resonant Case). In this subsection, we prove the existence of Arnold diffusion for a perturbed DNLS when $N = 3$, which is a 5-dimensional system. For arbitrary N, one can find large enough annular region inside the invariant plane Π (2.8), which is normally hyperbolic, for which the current proof can be easily applied. The point is that increasing unstable and stable dimensions does not pose substantial computational difficulty to establishing Arnold diffusion, while increasing the dimensions of tori does. We will study here the case that there is no resonance ($\omega = 0$) inside the invariant plane Π (2.8). The resonant case ($\omega \neq 0$) will be studied in next subsection.

Consider the following perturbation of the DNLS (2.1)

$$H = H_0 + \epsilon H_1 \ ,$$

where

$$H_1 = \alpha \sin t \sum_{n=0}^{N-1} \left| \frac{q_n - q_{n-1}}{h} \right|^2 + \sum_{n=0}^{N-1} \left[\left(\frac{q_n - q_{n-1}}{h} \right)^2 + \left(\frac{\overline{q_n} - \overline{q_{n-1}}}{h} \right)^2 \right] \ ,$$

where α is a real parameter. Under this perturbation, dynamics inside Π is unchanged. Π consists of periodic orbits forming concentric circles (2.9) [Figure 1]. We are interested in the following normally hyperbolic annular region inside Π

$$\mathcal{A} = \left\{ \vec{q} \in \Pi \mid \quad q_n = q, \ \forall n, \quad 3 \tan \frac{\pi}{3} < |q| < B \right\}$$

where B is an arbitrary large constant. Denote by $\{\mathcal{F}^{u,s}(\vec{q}) : \ \vec{q} \in \mathcal{A}\}$ the C^1 families of C^2 one dimensional unstable and stable Fenichel fibers with base points in $\mathcal{A}$ [**19**] such that for any $\vec{q}_* \in \mathcal{F}^u(\vec{q})$ or $\vec{q}_* \in \mathcal{F}^s(\vec{q})$, ($\vec{q} \in \mathcal{A}$),

$$\|F^t(\vec{q}_*) - \vec{q}\| \leq C e^{\kappa t} \|\vec{q}_* - \vec{q}\| \ , \quad \forall t \in (-\infty, 0] \ ,$$

or

$$\|F^t(\vec{q}_*) - \vec{q}\| \leq C e^{-\kappa t} \|\vec{q}_* - \vec{q}\| \ , \quad \forall t \in [0, \infty) \ ,$$

where F^t is the evolution operator of the perturbed DNLS, κ and C are some positive constants. The Fenichel fibers are C^1 in $\epsilon \in [0, \epsilon_0)$ for some $\epsilon_0 > 0$. It turns out that the constant of motion of DNLS (2.1)

$$I = \frac{1}{h^2} \sum_{n=0}^{N-1} \ln \rho_n$$

and F_1 [cf: (2.6) and (2.12)] are the best choices to build the two Melnikov-Arnold intergals. Restricted to Π,

$$I = \frac{1}{h^3} \ln \rho \ , \quad \rho = 1 + h^2 |q|^2 \ .$$

The level sets of I lead to all the periodic orbits (1-tori) in Π. The unstable and stable manifolds of an 1-torus given by $I = A$ (a constant) in $\mathcal{A}$ are

$$W^{u,s}(A) = \bigcup_{\vec{q} \in \mathcal{A}, \ I(\vec{q}) = A} \mathcal{F}^{u,s}(\vec{q}) \ ,$$

which are three dimensional (taking into account the time dimension).

Theorem 3.6 (Arnold Diffusion). *For any A_1 and A_2 such that*

$$\frac{1}{h^3} \ln \rho_0 < A_1 < A_2 < +\infty \ ,$$

where $\rho_0 = 1 + h^2\left(3\tan\frac{\pi}{3}\right)^2$, *there exists a* $\alpha_0 > 0$ *such that when* $|\alpha| > \alpha_0$, $W^u(A_1)$ *and* $W^s(A_2)$ *are connected by an orbit.*

PROOF. One can check directly that for any $\vec{q} \in \mathcal{A}$, $F_1(\vec{q}) = -2$ and $\partial F_1(\vec{q})/\partial \vec{q} = 0$ [cf: (2.6) and (2.12)]. Now consider $W^s(a_1)$ and $W^u(a_2)$. Along any orbit $\vec{q}^{\,s}(t)$ in $W^s(a_1)$, we have

$$\lim_{t\to+\infty} F_1(\vec{q}^{\,s}(t)) - F_1(\vec{q}^{\,s}(t)) = -2 - F_1(\vec{q}^{\,s}(t))$$
$$= \int_t^{+\infty} \frac{dF_1}{dt} dt = -i\epsilon \int_t^{+\infty} \{F_1, H_1\} dt \ ,$$
$$\lim_{t\to+\infty} I(\vec{q}^{\,s}(t)) - I(\vec{q}^{\,s}(t)) = a_1 - I(\vec{q}^{\,s}(t))$$
$$= \int_t^{+\infty} \frac{dI}{dt} dt = -i\epsilon \int_t^{+\infty} \{I, H_1\} dt \ ,$$

where

$$\{f, g\} = \sum_{n=0}^{N-1} \rho_n \left[\frac{\partial f}{\partial q_n} \frac{\partial g}{\partial \overline{q_n}} - \frac{\partial f}{\partial \overline{q_n}} \frac{\partial g}{\partial q_n} \right]$$

is the Poisson bracket. Notice that $\{F_1, H_0\} = \{I, H_0\} = 0$ at any $\vec{q} \in \mathcal{S}$. Since $\partial H_1/\partial \vec{q} \to 0$ exponentially as $t \to +\infty$, the corresponding integrals converge. Similarly along any orbit $\vec{q}^{\,u}(t)$ in $W^u(a_2)$, we have

$$F_1(\vec{q}^{\,u}(t)) - \lim_{t\to-\infty} F_1(\vec{q}^{\,u}(t)) = F_1(\vec{q}^{\,u}(t)) + 2$$
$$= \int_{-\infty}^{t} \frac{dF_1}{dt} dt = -i\epsilon \int_{-\infty}^{t} \{F_1, H_1\} dt \ ,$$
$$I(\vec{q}^{\,u}(t)) - \lim_{t\to-\infty} I(\vec{q}^{\,u}(t)) = I(\vec{q}^{\,u}(t)) - a_2$$
$$= \int_{-\infty}^{t} \frac{dI}{dt} dt = -i\epsilon \int_{-\infty}^{t} \{I, H_1\} dt \ .$$

Thus a neighborhood of $W^s(a_1)$ in $\mathcal{S}$ can be parameterized by (γ, t_0, t, F_1, I) where γ is defined in (2.9), t_0 is the initial time, and

$$F_1 = F_1(\vec{q}^{\,s}(t)) + v_1^s \ , \quad I = I(\vec{q}^{\,s}(t)) + v_2^s \ .$$

When $v_1^s = v_2^s = 0$, we get $W^s(a_1)$. Thus $W^s(a_1) \cap W^u(a_2) \neq \emptyset$ if and only if

$$F_1(\vec{q}^{\,s}(t)) = F_1(\vec{q}^{\,u}(t)) \ , \quad I(\vec{q}^{\,s}(t)) = I(\vec{q}^{\,u}(t)) \ ,$$

for some γ and t_0. In such a case, there is an orbit $\vec{q}(t,\epsilon) \subset W^s(a_1) \cap W^u(a_2)$ along which

$$\int_{-\infty}^{+\infty} \{F_1, H_1\}|_{\vec{q}(t,\epsilon)} dt = 0 \ , \quad a_1 - a_2 = -i\epsilon \int_{-\infty}^{+\infty} \{I, H_1\}|_{\vec{q}(t,\epsilon)} dt \ .$$

Let $\vec{q}(t, 0)$ be an orbit of DNLS such that $\vec{q}(0,0)$ and $\vec{q}(0,\epsilon)$ have the same stable fiber base point. Then

$$\|\vec{q}(0,0) - \vec{q}(0,\epsilon)\| \sim \mathcal{O}(\epsilon) \ .$$

For any small $\delta > 0$, there is a $T > 0$ such that

$$\left| \int_{\pm\infty}^{\pm T} \{F_1, H_1\}|_{\vec{q}(t,\epsilon)} dt \right| < \delta \ , \quad \left| \int_{\pm\infty}^{\pm T} \{I, H_1\}|_{\vec{q}(t,\epsilon)} dt \right| < \delta \ , \quad \forall \epsilon \in [0, \epsilon_0] \ ,$$

for some $\epsilon_0 > 0$. For this T, when ϵ is sufficiently small,

$$\|\vec{q}(t,0) - \vec{q}(t,\epsilon)\| \sim \mathcal{O}(\epsilon) \ , \quad \forall t \in [-T,T] \ .$$

Thus

$$\int_{-T}^{+T} \{F_1, H_1\}|_{\vec{q}(t,\epsilon)} dt = \int_{-T}^{+T} \{F_1, H_1\}|_{\vec{q}(t,0)} dt + \mathcal{O}(\epsilon) \ ,$$
$$\int_{-T}^{+T} \{I, H_1\}|_{\vec{q}(t,\epsilon)} dt = \int_{-T}^{+T} \{I, H_1\}|_{\vec{q}(t,0)} dt + \mathcal{O}(\epsilon) \ .$$

Finally we have

$$\int_{-\infty}^{+\infty} \{F_1, H_1\}|_{\vec{q}(t,\epsilon)} dt = \int_{-\infty}^{+\infty} \{F_1, H_1\}|_{\vec{q}(t,0)} dt + \mathcal{O}(\delta) = 0 \ , \tag{3.2}$$

$$a_1 - a_2 = -i\epsilon \int_{-\infty}^{+\infty} \{I, H_1\}|_{\vec{q}(t,\epsilon)} dt = -i\epsilon \int_{-\infty}^{+\infty} \{I, H_1\}|_{\vec{q}(t,0)} dt + \mathcal{O}(\delta\epsilon) \ . \tag{3.3}$$

Next we solve the above equations at the leading order in δ and ϵ. Rewrite the derivative given in (2.12) as follows

$$\partial F_1 / \partial q_n = V_n e^{-i\hat{\gamma}} \ ,$$

where $\hat{\gamma} = \gamma + 2(a^2 - \omega^2)t_0$, $t_0 = p/\mu$, and V_n represents the rest which does not depend on $\hat{\gamma}$. We also rewrite q_c (2.9) and q_n (2.11) as

$$q_c = \hat{q}_c e^{i\hat{\gamma}} \ , \quad q_n = \hat{q}_n e^{i\hat{\gamma}} \ ,$$

where $\hat{q}_c$ and $\hat{q}_n$ do not depend on $\hat{\gamma}$. Then substitute all these into the leading order terms in (3.2)-(3.3), we obtain the following equations

$$\alpha\sqrt{M_1^2 + M_2^2}\sin(t_0 + \theta_1) + \sqrt{M_3^2 + M_4^2}\sin(2\hat{\gamma} + \theta_2) = 0 \ , \tag{3.4}$$

$$a_1 - a_2 = 2\epsilon\sqrt{M_5^2 + M_6^2}\sin(2\hat{\gamma} + \theta_3) \ , \tag{3.5}$$

where

$$\cos\theta_1 = \frac{M_1}{\sqrt{M_1^2+M_2^2}}\ , \quad \sin\theta_1 = \frac{M_2}{\sqrt{M_1^2+M_2^2}}\ , \quad \cos\theta_2 = \frac{M_3}{\sqrt{M_3^2+M_4^2}}\ ,$$

$$\sin\theta_2 = \frac{M_4}{\sqrt{M_3^2+M_4^2}}\ , \quad \cos\theta_3 = \frac{M_5}{\sqrt{M_5^2+M_6^2}}\ , \quad \sin\theta_3 = \frac{M_6}{\sqrt{M_5^2+M_6^2}}\ ,$$

$$M_1 = \int_{-\infty}^{+\infty}\sum_{n=0}^{N-1}\cos\tau\ \rho_n\ \mathrm{Im}\ [V_n G_n^1]\ d\tau\ ,$$

$$M_2 = -\int_{-\infty}^{+\infty}\sum_{n=0}^{N-1}\sin\tau\ \rho_n\ \mathrm{Im}\ [V_n G_n^1]\ d\tau\ ,$$

$$M_3 = \int_{-\infty}^{+\infty}\sum_{n=0}^{N-1}\rho_n\ \mathrm{Re}\ [V_n G_n^2]\ d\tau\ , \quad M_4 = -\int_{-\infty}^{+\infty}\sum_{n=0}^{N-1}\rho_n\ \mathrm{Im}\ [V_n G_n^2]\ d\tau\ ,$$

$$M_5 = -\int_{-\infty}^{+\infty}\sum_{n=0}^{N-1}\mathrm{Re}\ G_n^3\ d\tau\ , \quad M_6 = \int_{-\infty}^{+\infty}\sum_{n=0}^{N-1}\mathrm{Im}\ G_n^3\ d\tau\ ,$$

$$G_n^1 = \frac{\hat{q}_{n+1} - 2\hat{q}_n + \hat{q}_{n-1}}{h^2}\ , \quad G_n^2 = 2\frac{\overline{\hat{q}_{n+1}} - 2\overline{\hat{q}_n} + \overline{\hat{q}_{n-1}}}{h^2}\ ,$$

$$G_n^3 = -2\frac{\overline{\hat{q}_n}(\overline{\hat{q}_{n+1}} - 2\overline{\hat{q}_n} + \overline{\hat{q}_{n-1}})}{h^2}\ ,$$

and $\tau = t + p/\mu$. Equations (3.4)-(3.5) are easily solvable as long as neither $\sqrt{M_1^2+M_2^2}$ nor $\sqrt{M_5^2+M_6^2}$ vanishes. In Figures 2-4, we plot the graphs of them as functions of a. We solve equation (3.5) for $\hat{\gamma}$, then solve equation (3.4) for t_0. Thus when $|\alpha|$ is large enough, we have solutions. It is also clear from equations (3.4)-(3.5) that $W^s(a_1)$ and $W^u(a_2)$ intersect transversally. Then we can choose a sequence

$$A_1 = a_1 < a_2 < \cdots < a_N = A_2\ ,$$

such that $W^s(a_j)$ and $W^u(a_{j+1})$ $(1 \le j \le N-1)$ intersect transversally. The period of the 1-tori (2.9) is π/a^2. Thus we can always choose the a_j's such that the frequencies $\frac{1}{2a^2}$ of the corresponding 1-tori are irrational. Therefore we obtain a transition chain. Apply Lemma 3.4 to the period-2π map of the DNLS, we obtain the claim of the theorem. □

REMARK 3.7. The constant of motion I is equivalent to F_2 for $z_2^c = 1$ (2.6). The continuum limit of H_1 has the form

$$H_1 = \alpha\sin t\int_0^1 |q_x|^2 dx + \int_0^1 (q_x^2 + \overline{q_x}^{\ 2})dx\ ,$$

which is suitable for the NLS setting. One can regularize the perturbation by replacing the partial derivative ∂_x in H_1 by a Fourier multiplier $\hat{\partial}_x$, e.g. a Galerkin truncation. One can use the constant of motion

$$I = \int_0^1 |q|^2 dx$$

to build the second Melnikov-Arnold integral.

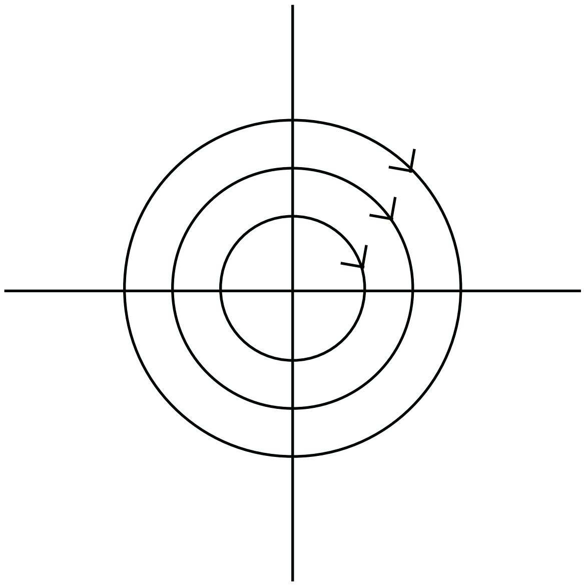

FIGURE 1. Dynamics inside Π (non-resonant case).

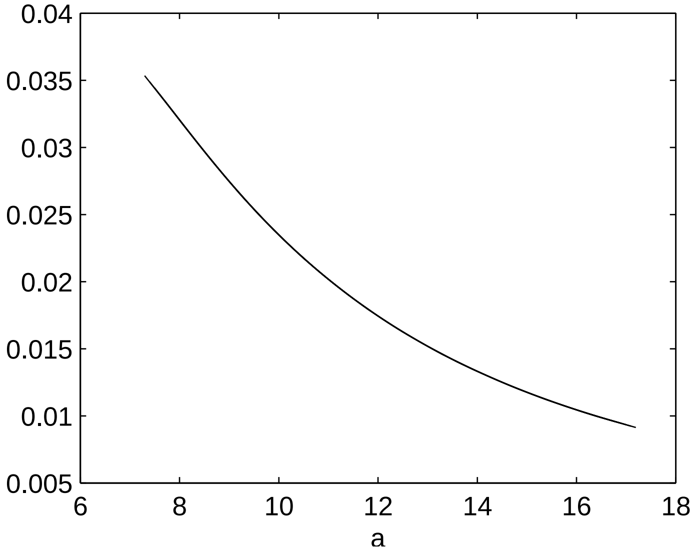

FIGURE 2. The graph of $\sqrt{M_1^2 + M_2^2}$ as a function of a in the non-resonant case $\omega = 0$.

3.2. Arnold Diffusion of DNLS ($N = 3$, Resonant Case). In this subsection, we prove the existence of Arnold diffusion for a perturbed DNLS when $N = 3$, which is a 5-dimensional system. We will study here the case that there is a resonance ($\omega > 3 \tan \frac{\pi}{3}$) inside the invariant plane Π (2.8).

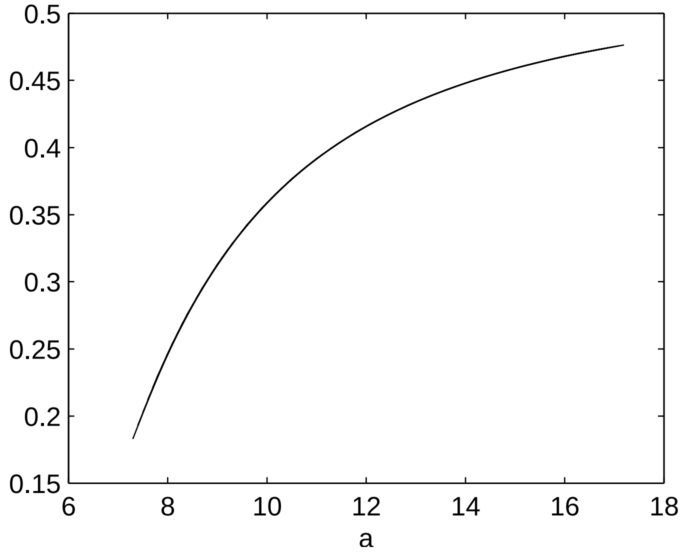

FIGURE 3. The graph of $\sqrt{M_3^2 + M_4^2}$ as a function of a in the non-resonant case $\omega = 0$.

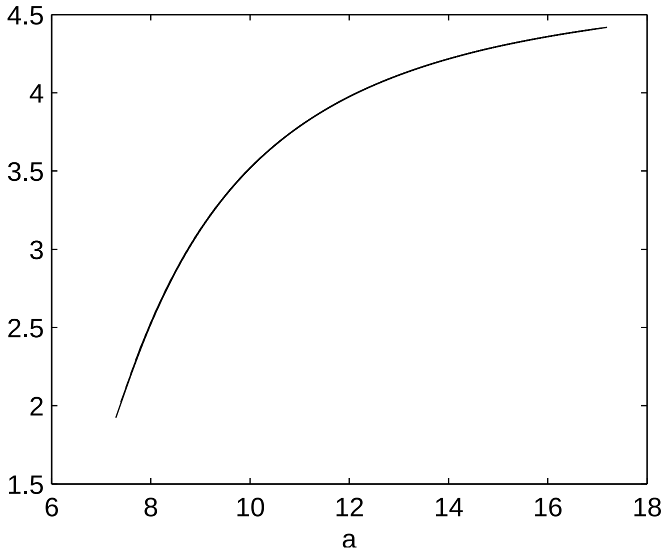

FIGURE 4. The graph of $\sqrt{M_5^2 + M_6^2}$ as a function of a in the non-resonant case $\omega = 0$.

Consider the following perturbation of the DNLS (2.1)

$$H = H_0 + \epsilon(H_1 + H_2) ,$$

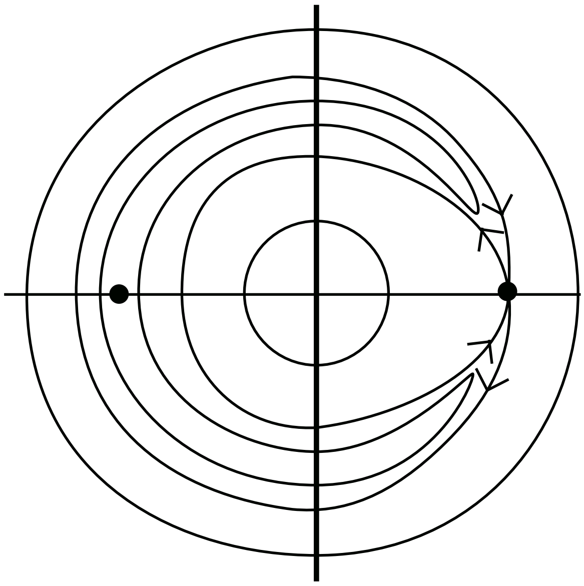

FIGURE 5. Dynamics inside Π (resonant case).

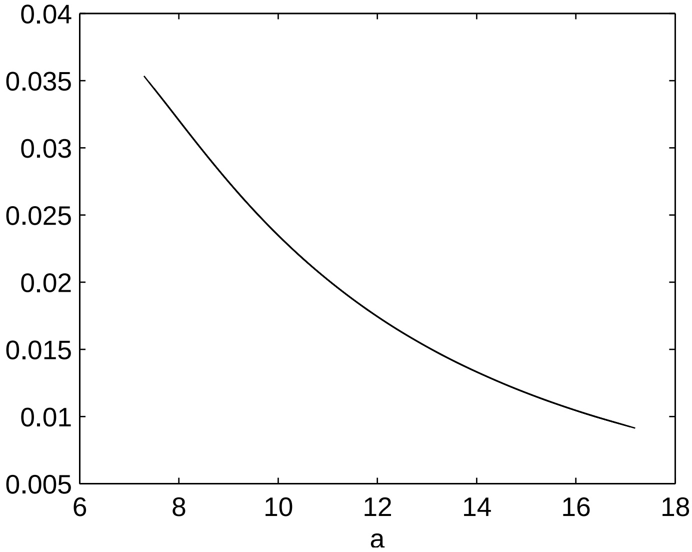

FIGURE 6. The graph of $\sqrt{M_1^2 + M_2^2}$ as a function of a in the resonant case $\omega = 10$.

where

$$H_1 = \alpha \sum_{n=0}^{N-1} (q_n + \overline{q_n}) \ , \quad H_2 = \sin t \sum_{n=0}^{N-1} \left| \frac{q_n - q_{n-1}}{h} \right|^2 \ ,$$

where α is a real parameter. Under this perturbation, dynamics inside Π is changed. Due to the resonance $a = \omega$ in (2.9), some tori do not persist into KAM tori. A

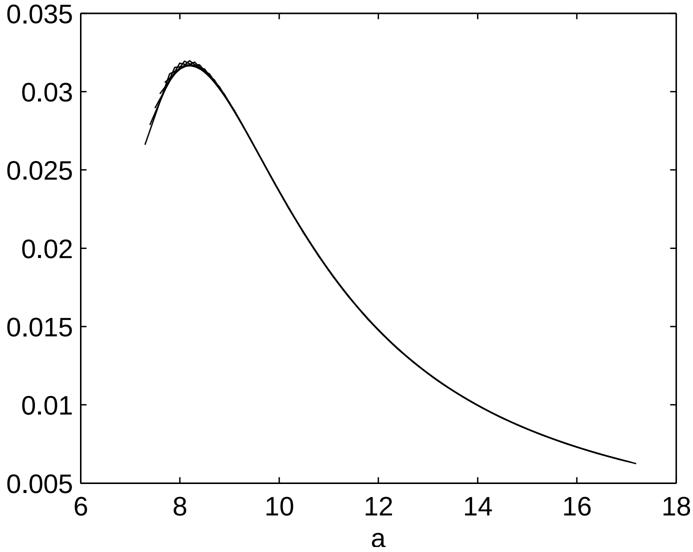

FIGURE 7. The graph of $\sqrt{M_3^2 + M_4^2}$ as a function of a in the resonant case $\omega = 10$.

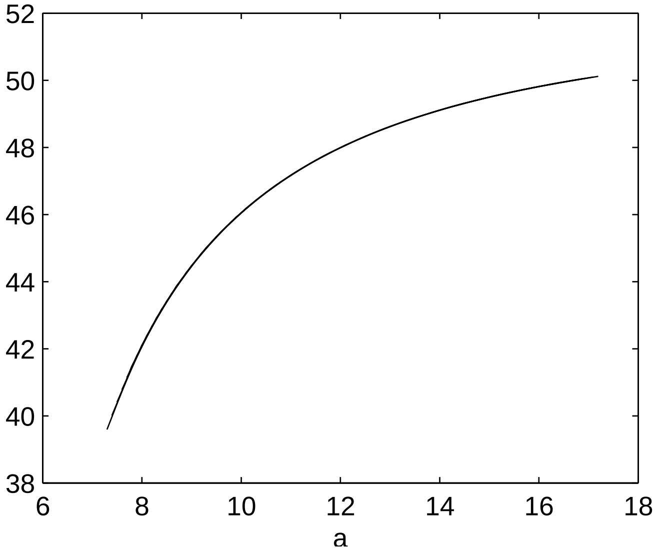

FIGURE 8. The graph of $\sqrt{M_5^2 + M_6^2}$ as a function of a in the resonant case $\omega = 10$.

secondary separatrix is generated. Inside this separatrix are the secondary tori [Figure 5]. As can be seen below, resonance does not add difficulty to the Arnold diffusion problem. Instead of I in last subsection, we use

$$\hat{H} = H = H_0 + \epsilon H_1 \ ,$$

to build one of the two Melnikov-Arnold integrals. Restricted to Π, the level sets of $\hat{H}$ produces Figure 5. The unstable and stable manifolds of an 1-torus given by $\hat{H} = A$ (a constant) in $\mathcal{A}$ are

$$W^{u,s}(A) = \bigcup_{\vec{q}\in\mathcal{A},\ \hat{H}(\vec{q})=A} \mathcal{F}^{u,s}(\vec{q}) \ .$$

Let

$$A_* = \frac{1}{h^3}\left[2\left(3\tan\frac{\pi}{3}\right)^2 - \frac{2}{h^2}(1+\omega^2h^2)\ln\rho_0\right] \ ,$$

where $\rho_0 = 1 + h^2\left(3\tan\frac{\pi}{3}\right)^2$.

Theorem 3.8 (Arnold Diffusion). *For any A_1 and A_2 such that*

$$A_* < A_1 < A_2 < +\infty \ ,$$

there exists a $\alpha_0 > 0$ such that when $|\alpha| > \alpha_0$, $W^u(A_1)$ and $W^s(A_2)$ are connected by an orbit.

Proof. Again one can check directly that for any $\vec{q} \in \mathcal{A}$, $F_1(\vec{q}) = -2$ and $\partial F_1(\vec{q})/\partial\vec{q} = 0$ [cf: (2.6) and (2.12)]. Similar to the proof of Theorem 3.6, consider $W^s(a_1)$ and $W^u(a_2)$. Along any orbit $\vec{q}^{\,s}(t)$ in $W^s(a_1)$, we have

$$\lim_{t\to+\infty} F_1(\vec{q}^{\,s}(t)) - F_1(\vec{q}^{\,s}(t)) = -2 - F_1(\vec{q}^{\,s}(t))$$
$$= \int_t^{+\infty} \frac{dF_1}{dt}dt = -i\epsilon\int_t^{+\infty}\{F_1, H_1 + H_2\}dt \ ,$$
$$\lim_{t\to+\infty} \hat{H}(\vec{q}^{\,s}(t)) - \hat{H}(\vec{q}^{\,s}(t)) = a_1 - \hat{H}(\vec{q}^{\,s}(t))$$
$$= \int_t^{+\infty} \frac{d\hat{H}}{dt}dt = -i\epsilon\int_t^{+\infty}\{\hat{H}, H_2\}dt \ ,$$

where

$$\{f,g\} = \sum_{n=0}^{N-1}\rho_n\left[\frac{\partial f}{\partial q_n}\frac{\partial g}{\partial \overline{q_n}} - \frac{\partial f}{\partial \overline{q_n}}\frac{\partial g}{\partial q_n}\right]$$

is the Poisson bracket. Notice that $\{F_1, H_0\} = \{\hat{H}, \hat{H}\} = 0$ at any $\vec{q} \in \mathcal{S}$. Since $\frac{\partial F_1}{\partial \vec{q}}, \frac{\partial H_2}{\partial \vec{q}} \to 0$ exponentially as $t \to +\infty$, the corresponding integrals converge. Similarly along any orbit $\vec{q}^{\,u}(t)$ in $W^u(a_2)$, we have

$$F_1(\vec{q}^{\,u}(t)) - \lim_{t\to-\infty} F_1(\vec{q}^{\,u}(t)) = F_1(\vec{q}^{\,u}(t)) + 2$$
$$= \int_{-\infty}^{t} \frac{dF_1}{dt}dt = -i\epsilon\int_{-\infty}^{t}\{F_1, H_1 + H_2\}dt \ ,$$
$$\hat{H}(\vec{q}^{\,u}(t)) - \lim_{t\to-\infty} \hat{H}(\vec{q}^{\,u}(t)) = \hat{H}(\vec{q}^{\,u}(t)) - a_2$$
$$= \int_{-\infty}^{t} \frac{d\hat{H}}{dt}dt = -i\epsilon\int_{-\infty}^{t}\{\hat{H}, H_2\}dt \ .$$

Thus a neighborhood of $W^s(a_1)$ in $\mathcal{S}$ can be parameterized by $(\vartheta, t_0, t, F_1, \hat{H})$ where ϑ is the angle of the 1-torus $\hat{H} = a_1$ in Π, t_0 is the initial time, and

$$F_1 = F_1(\vec{q}^{\,s}(t)) + v_1^s \ , \quad \hat{H} = \hat{H}(\vec{q}^{\,s}(t)) + v_2^s \ .$$

When $v_1^s = v_2^s = 0$, we get $W^s(a_1)$. Thus $W^s(a_1) \cap W^u(a_2) \neq \emptyset$ if and only if

$$F_1(\vec{q}^{\,s}(t)) = F_1(\vec{q}^{\,u}(t)) \ , \quad \hat{H}(\vec{q}^{\,s}(t)) = \hat{H}(\vec{q}^{\,u}(t)) \ ,$$

for some ϑ and t_0. In such a case, there is an orbit $\vec{q}(t,\epsilon) \subset W^s(a_1) \cap W^u(a_2)$ along which

$$\int_{-\infty}^{+\infty} \{F_1, H_1 + H_2\}|_{\vec{q}(t,\epsilon)} dt = 0 \ , \quad a_1 - a_2 = -i\epsilon \int_{-\infty}^{+\infty} \{\hat{H}, H_2\}|_{\vec{q}(t,\epsilon)} dt \ .$$

Let $\vec{q}(t,0)$ be an orbit of DNLS such that $\vec{q}(0,0)$ and $\vec{q}(0,\epsilon)$ have the same stable fiber base point. Then

$$\|\vec{q}(0,0) - \vec{q}(0,\epsilon)\| \sim \mathcal{O}(\epsilon) \ .$$

For any small $\delta > 0$, there is a $T > 0$ such that

$$\left| \int_{\pm\infty}^{\pm T} \{F_1, H_1 + H_2\}|_{\vec{q}(t,\epsilon)} dt \right| < \delta \ , \quad \left| \int_{\pm\infty}^{\pm T} \{\hat{H}, H_2\}|_{\vec{q}(t,\epsilon)} dt \right| < \delta \ , \quad \forall \epsilon \in [0, \epsilon_0] \ ,$$

for some $\epsilon_0 > 0$. For this T, when ϵ is sufficiently small,

$$\|\vec{q}(t,0) - \vec{q}(t,\epsilon)\| \sim \mathcal{O}(\epsilon) \ , \quad \forall t \in [-T, T] \ .$$

Thus

$$\int_{-T}^{+T} \{F_1, H_1 + H_2\}|_{\vec{q}(t,\epsilon)} dt = \int_{-T}^{+T} \{F_1, H_1 + H_2\}|_{\vec{q}(t,0)} dt + \mathcal{O}(\epsilon) \ ,$$
$$\int_{-T}^{+T} \{\hat{H}, H_2\}|_{\vec{q}(t,\epsilon)} dt = \int_{-T}^{+T} \{\hat{H}, H_2\}|_{\vec{q}(t,0)} dt + \mathcal{O}(\epsilon) \ .$$

Finally we have

$$\int_{-\infty}^{+\infty} \{F_1, H_1 + H_2\}|_{\vec{q}(t,\epsilon)} dt = \int_{-\infty}^{+\infty} \{F_1, H_1 + H_2\}|_{\vec{q}(t,0)} dt + \mathcal{O}(\delta) = 0 \ , \tag{3.6}$$

$$a_1 - a_2 = -i\epsilon \int_{-\infty}^{+\infty} \{\hat{H}, H_2\}|_{\vec{q}(t,\epsilon)} dt = -i\epsilon \int_{-\infty}^{+\infty} \{H_0, H_2\}|_{\vec{q}(t,0)} dt + \mathcal{O}(\delta\epsilon) \ . \tag{3.7}$$

To the leading order terms in (3.6)-(3.7), we obtain the following equations

$$\sqrt{M_1^2 + M_2^2} \sin(t_0 + \theta_1) + \alpha \sqrt{M_3^2 + M_4^2} \sin(\hat{\gamma} + \theta_2) = 0 \ , \tag{3.8}$$

$$a_1 - a_2 = 2\epsilon \sqrt{M_5^2 + M_6^2} \sin(t_0 + \theta_3) \ , \tag{3.9}$$

where

$$\cos\theta_1 = \frac{M_1}{\sqrt{M_1^2+M_2^2}} \ , \quad \sin\theta_1 = \frac{M_2}{\sqrt{M_1^2+M_2^2}} \ , \quad \cos\theta_2 = \frac{M_3}{\sqrt{M_3^2+M_4^2}} \ ,$$

$$\sin\theta_2 = \frac{M_4}{\sqrt{M_3^2+M_4^2}} \ , \quad \cos\theta_3 = \frac{M_5}{\sqrt{M_5^2+M_6^2}} \ , \quad \sin\theta_3 = \frac{M_6}{\sqrt{M_5^2+M_6^2}} \ ,$$

$$M_1 = \int_{-\infty}^{+\infty} \sum_{n=0}^{N-1} \cos\tau \ \rho_n \ \text{Im}\ [V_n G_n^1] \ d\tau \ ,$$

$$M_2 = -\int_{-\infty}^{+\infty} \sum_{n=0}^{N-1} \sin\tau \ \rho_n \ \text{Im}\ [V_n G_n^1] \ d\tau \ ,$$

$$M_3 = -\int_{-\infty}^{+\infty} \sum_{n=0}^{N-1} \rho_n \ \text{Re}\ [V_n] \ d\tau \ , \quad M_4 = \int_{-\infty}^{+\infty} \sum_{n=0}^{N-1} \rho_n \ \text{Im}\ [V_n] \ d\tau \ ,$$

$$M_5 = \int_{-\infty}^{+\infty} \sum_{n=0}^{N-1} \cos\tau \ \text{Im}\ [G_n^1 G_n^2] \ d\tau \ ,$$

$$M_6 = -\int_{-\infty}^{+\infty} \sum_{n=0}^{N-1} \sin\tau \ \text{Im}\ [G_n^1 G_n^2] \ d\tau \ ,$$

$$G_n^1 = \frac{\hat{q}_{n+1} - 2\hat{q}_n + \hat{q}_{n-1}}{h^2} \ ,$$

$$G_n^2 = \frac{1}{h^2}\left[\overline{\hat{q}_{n+1}} - 2\overline{\hat{q}_n} + \overline{\hat{q}_{n-1}}\right] + |\hat{q}_n|^2 \left[\overline{\hat{q}_{n+1}} + \overline{\hat{q}_{n-1}}\right] - 2\omega^2 \overline{\hat{q}_n} \ ,$$

and $\tau = t + p/\mu$. Equations (3.8)-(3.9) are easily solvable as long as neither $\sqrt{M_3^2+M_4^2}$ nor $\sqrt{M_5^2+M_6^2}$ vanishes. In Figures 6-8, we plot the graphs of them as functions of a. We solve equation (3.9) for t_0, then solve equation (3.8) for $\hat{\gamma}$. Thus when $|\alpha|$ is large enough, we have solutions. It is also clear from equations (3.8)-(3.9) that $W^s(a_1)$ and $W^u(a_2)$ intersect transversally. Then we can choose a sequence

$$A_1 = a_1 < a_2 < \cdots < a_N = A_2 \ ,$$

such that $W^s(a_j)$ and $W^u(a_{j+1})$ $(1 \le j \le N-1)$ intersect transversally. The period of the 1-tori $(\hat{H} = a_j)$ depends on a_j no matter they are KAM tori or secondary tori. We can always choose the a_j's such that the frequencies of the corresponding 1-tori are irrational. We can use one secondary torus inside and close enough to the separatrix (Figure 5) to bridge across the resonant region of width $\mathcal{O}(\sqrt{\epsilon})$. Therefore we obtain a transition chain. Apply Lemma 3.4 to the period-2π map of the DNLS, we obtain the claim of the theorem. □

Remark 3.9. The continuum limit of H_1 and H_2 have the form

$$H_1 = \alpha \int_0^1 (q+\bar{q})dx \ , \quad H_2 = \sin t \int_0^1 |q_x|^2 dx \ ,$$

which is suitable for the NLS setting. One can regularize the perturbation by replacing the partial derivative ∂_x in H_2 by a Fourier multiplier $\hat{\partial}_x$, e.g. a Galerkin truncation.

References

[1] M. Ablowitz, J. Ladik, A nonlinear difference scheme and inverse scattering, *Studies in Appl. Math.* **55** (1976), 213-229.

[2] M. Ablowitz, B. Prinari, A. Trubatch, *Discrete and Continuous Nonlinear Schrödinger Systems*, Cambridge University Press, 2004.

[3] V. Arnold, Instability of dynamical systems with several degrees of freedom, *Soviet Math. Doklady* **5** (1964), 581-585.

[4] V. Arnold, A. Avez, *Ergodic Problems of Classical Mechanics*, W. A. Benjamin, Inc., New York, 1968. [Page 112, Lemma 23.8]

[5] M. Berti, L. Biasco, P. Bolle, Drift in phase space: a new variational mechanism with optimal diffusion time, *J. Math. Pures Appl.* **82, no.6** (2003), 613-664.

[6] S. Bolotin, D. Treschev, Unbounded growth of energy in nonautonomous Hamiltonian systems, *Nonlinearity* **12** (1999), 365-388.

[7] C. Cheng, J. Yan, Existence of diffusion orbits in a priori unstable Hamiltonian systems, *J. Diff. Geom.* **67, no.3** (2004), 457-517.

[8] L. Chierchia, G. Gallavotti, Drift and diffusion in phase space, *Ann. Inst. H. Poincaré Phys. Theor.* **60** (1994), 1-144.

[9] L. Chierchia, E. Valdinoci, A note on the construction of Hamiltonian trajectories along heteroclinic chains, *Forum Math.* **12** (2000), 247-255.

[10] J. Cresson, A λ-lemma for partially hyperbolic tori and the obstruction property, *Lett. Math. Phys.* **42** (1997), 363-377.

[11] A. Delshams, R. de la Llave, T. Seara, A geometric mechanism for diffusion in Hamiltonian systems overcoming the large gap problem: Heuristics and rigorous verification on a model, *Memoirs of AMS* **179, no.844** (2006).

[12] A. Delshams, R. de la Llave, T. Seara, A geometric approach to the existence of orbits with unbounded energy in generic periodic perturbations by potential of generic geodesic flows on $\mathbb{T}^2$, *Comm. Math. Phys.* **209** (2000), 353-392.

[13] R. Douady, Stabilité ou instabilité des points fixes elliptiques, *Ann Sci. de l'ENS* **21** (1988), 1-46.

[14] E. Fontich, P. Martin, Differentiable invariant manifolds for partially hyperbolic tori and a lambda lemma, *Nonlinearity* **13** (2000), 1561-1593. [Page 1585]

[15] E. Fontich, P. Martin, Hamiltonian systems with orbits covering densely submanifolds of small codimension, *Nonlinear Analysis* **52** (2003), 315-327.

[16] R. de la Llave, C.E. Wayne, Whiskered and low dimensional tori in nearly integrable Hamiltonian systems, *Math. Phys. Electron. J.* **10** (2004), paper 5, 45pp.

[17] Y. Li, Bäcklund transformations and homoclinic structures for the discrete NLS equation, *Phys. Lett. A* **163** (1992), 181-187.

[18] Y. Li, Homoclinic tubes in discrete nonlinear Schrödinger equation under Hamiltonian perturbations, *Nonlinear Dynamics* **vol.31, no.4** (2003), 393-434.

[19] Y. Li, *Chaos in Partial Differential Equations*, International Press, 2004.

[20] Y. Li, Homoclinic tubes in nonlinear Schrödinger equation under Hamiltonian perturbations, *Progr. Theoret. Phys.* **101, no.3** (1999), 559-577.

[21] Y. Li, Persistent homoclinic orbits of nonlinear Schrödinger equation under singular perturbations, *Dynamics of PDE* **1, no.1** (2004), 87-123.

[22] Y. Li, Existence of chaos for nonlinear Schrödinger equation under singular perturbations, *Dynamics of PDE* **1, no.2** (2004), 225-237.

[23] Y. Li, Chaos and shadowing lemma for autonomous systems of infinite dimensions, *J. Dyn. Diff. Eq.* **vol.15, no.4** (2003), 699-730. [Page 705]

[24] Y. Li, Chaos and shadowing around a homoclinic tube, *Abstract and Applied Analysis* **vol.2003, no.16** (2003), 923-931.

[25] Y. Li, Homoclinic tubes and chaos in perturbed Sine-Gordon equation, *Chaos, Solitons and Fractals* **vol.20, no.4** (2004), 791-798.

[26] Y. Li, Chaos and shadowing around a heteroclinically tubular cycle with an application to sine-Gordon equation, *Studies in Appl. Math.* **116** (2006), 145-171.

[27] Y. Li, Tubes in dynamical systems, *http://www.math.missouri.edu/˜cli* (2006), Submitted.

[28] J. Marco, Transition le long des chaînes de tores invariants pour les systèmes Hamiltoniens analytiques, *Ann. Inst. H. Poincaré* **64** (1996), 205-252.

[29] J. Mather, Arnold diffusion. I: Announcement of results, *J. Math. Sci.* **124, no.5** (2004), 5275-5289.

[30] P. Perfetti, Fixed point theorems in the Arnold model about instability of Hamiltonian dynamical systems, *Discrete Contin. Dynam. Syst.* **4** (1998), 379-391.

[31] Z. Xia, Arnold diffusion: a variational construction, *Proc. ICM* **vol.II** (1998), 867-877.

Department of Mathematics, University of Missouri, Columbia, MO 65211
E-mail address: cli@math.missouri.edu