Summer 2015

Preservation of Periodicity in Variational Integrators

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DOI: <https://doi.org/10.31979/etd.c4z9-y9yp>
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PRESERVATION OF PERIODICITY IN VARIATIONAL INTEGRATORS

A Thesis

Presented to

The Faculty of the Department of Mathematics

San José State University

In Partial Fulfillment

of the Requirements for the Degree

Master of Science

by

Jian-Long Liu

August 2015

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The Designated Thesis Committee Approves the Thesis Titled
PRESERVATION OF PERIODICITY IN VARIATIONAL INTEGRATORS

by

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APPROVED FOR THE DEPARTMENT OF MATHEMATICS

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August 2015

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ABSTRACT

PRESERVATION OF PERIODICITY IN VARIATIONAL INTEGRATORS

by Jian-Long Liu

Classical numerical integrators do not preserve symplecticity, a structure inherent in Hamiltonian systems. Thus, the trajectories they produce cannot be expected to possess the same qualitative behavior observed in the original system. Pooling recent results from O’Neale and West, we explore a particular class of numerical integrators, the *variational integrator*, that preserves one aspect of the range of behavior present in Hamiltonian systems, the periodicity of trajectories. We first establish the prerequisites and some key concepts from Hamiltonian systems, particularly symplecticity and action-angle coordinates. Through perturbation theory and its complications manifested in small divisor problems, we motivate the necessity for KAM theory. With O’Neale’s KAM-type theorem, we observe the preservation of periodicity by symplectic one-step methods. Lastly, we show that the variational integrator introduced by West possesses the defining characteristics of symplectic one-step methods, and therefore also preserves periodicity of the original trajectories.

ACKNOWLEDGEMENTS

I wish to express my sincerest gratitude to my thesis committee, particularly Prof. Slobodan Simić, without whose guidance and encouragements I would not have the appreciation of the subject of KAM theory and mathematics as a whole as I do today. I am also grateful for the advice provided by Dr. Dion Robert James O’Neale towards my understanding of KAM theory. I would also like to thank Prof. Jared Maruskin for his help in further developing my understanding of dynamical systems, and his inspiration for my initial foray into classical mechanics.

Finally, I would like to thank my family, particularly my parents, for their continual support, moral or otherwise. Without them, I would not have been able to accomplish the achievements I enjoy today.

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CHAPTER 1

INTRODUCTION

Most physical phenomena are described by continuous-time dynamical systems. In particular, of greatest interest to us is the class of Hamiltonian systems. These systems possess most of the features we wish to retain from the physical processes in the ideal setting. For example, if we are to study the evolution of celestial bodies, we would not attempt to record the spatial coordinates at numerous time instances. Rather, we would study the corresponding Hamiltonian system and how it has evolved with the progression of time.

Although writing down the set of rules governing the evolution of a system is somewhat straightforward, exploring and determining the range of motion are highly nontrivial tasks. In fact, there is no explicit solution describing the trajectories of celestial bodies even when we restrict the number of revolving objects to just three. Thus, many approaches to circumvent the need for explicit solution trajectories have been developed.

Applied mathematicians attempted to derive accurate numerical integrators to estimate the behavior of particular trajectories for a short time. Pure mathematicians looked for the portions of the phase space that remains invariant, regardless of the length of the time period. Although the answer to the classification of all of the solution trajectories is yet to be achieved, some recent results (e.g. [Wes04] and [O’N09]) using a mixture of the two branches have shown promise.

More specifically, there are types of numerical integrators that preserve periodicity of the trajectories from Hamiltonian systems. In other words, to question the periodicity of a particular trajectory, one can ask whether the corresponding discrete set of points produced by the numerical integrator is periodic or not. While the answer to this question

does not establish all of the sufficient conditions for the periodicity of the original trajectory, it gives us some basis for what to expect in the remaining conditions as well as where to start to classify the trajectories whose behaviors are vastly more complex.

The goal of this thesis was to derive a class of numerical integrators, the so-called variational integrators, following West ([Wes04]), to show that they preserve periodicity via a KAM-type theorem stated by O’Neale ([O’N09]), and to illustrate the results with some simple examples. Our main examples are the simple harmonic oscillator and the pendulum. They are introduced as we define Hamiltonian systems and will evolve in parallel to solidify our understanding of the theory, concluding with the results of applying the variational integrator to them.

We first explore most of the background required for Hamiltonian systems, along with the key feature of symplecticity, as well as the equivalence to Lagrangian systems. Next, we examine the motivation of Kolmogorov-Arnold-Moser (KAM) theory from classical perturbation theory, with a sketch of its proof that is, we believe, accessible and straightforward. Using KAM-type proofs, we then proceed to describe the results obtained by O’Neale ([O’N09]), wherein it can be shown that there exist numerical integrators that preserve periodicity of trajectories. Lastly, we delve into an intuitive way presented by West ([Wes04]), in which the variational integrator, an integrator of the type described by O’Neale, can be easily derived by utilizing the idea of symplecticity.

This paper is intended as a survey paper, where we sacrifice the intricate details for clarity and intuitiveness, to present the background leading up to the key theorems and to sketch how the theorems are proven.

We assume some background in manifolds and differential forms as well as knowledge in the basics of dynamical systems. For manifolds and differential forms, we recommend a standard text, *Introduction to Smooth Manifolds* ([Lee03]), whereas for dynamical systems, *Differential Equations, Dynamical Systems, and an Introduction to*

Chaos ([HSD04]) is sufficient. Although experience in classical mechanics is helpful in understanding the physical interpretation, it is not a requirement. The reader is welcome to delve into it in *Classical Mechanics* ([Gol02]).

CHAPTER 2

HAMILTONIAN SYSTEMS

Hamiltonian systems form a class of dynamical systems with features that mirror how physical phenomena evolve in an idealized world. Thus, our first topic of discussion is how they are defined. Rather than advancing along the historical progression of developing Hamiltonian systems from Lagrangian systems, we start with the definition of a symplectic manifold.

From there, we arrive naturally at the definition of Hamiltonian systems. Briefly touching on Liouville integrability and the action-angle transformation, we finish with the formulation of Lagrangian systems, via both Hamilton's principle and the (inverse) Legendre transform from Hamiltonian systems.

2.1 Symplecticity

Symplecticity is a concept central to Hamiltonian systems. We thus begin by introducing some basic ideas.

Definition 2.1.1. A *symplectic form* on an even-dimensional manifold is a skew-symmetric, nondegenerate, bilinear differential form. An even-dimensional manifold M equipped with a symplectic form ω , or (M, ω) , is called a *symplectic manifold*.

On a symplectic manifold, the coordinates are usually written as (q, p) , where q is called the *generalized position* and p is the *generalized momentum*, both of which are n -dimensional.

Example 2.1.2. A simple example of a symplectic form on $\mathbb{R}^{2n}$ is the *standard symplectic form*

$$\omega_0(u, v) = \langle u, Jv \rangle$$

for all $u, v \in \mathbb{R}^{2n}$, with

$$J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \quad (2.1)$$

and I_n the $n \times n$ identity matrix. □

Next, we introduce maps which preserve the symplectic structure.

Definition 2.1.3. Let (M, ω_M) and (N, ω_N) be n -dimensional symplectic manifolds. A *symplectic map*, or *canonical transformation*, is a diffeomorphism $f : M \rightarrow N$ such that, for all $u, v \in M$,

$$\omega_M(u, v) = \omega_N(df(u), df(v)), \quad (2.2)$$

where df is the differential of f .

Applying the definition directly to linear transformations on vector spaces, we have the following example.

Example 2.1.4. Let $(\mathbb{R}^{2n}, \omega)$ be a symplectic vector space. Let $T : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ be a linear transformation, with the corresponding matrix A relative to some basis. Then T preserves ω if

$$\omega(u, v) = \omega(T(u), T(v)),$$

which corresponds to

$$A^\top J A = J.$$

Thus T is a canonical transformation if and only if A satisfies this matrix equation. □

This example motivates the definition of a symplectic matrix.

Definition 2.1.5. Let $A \in \mathbb{R}^{2n \times 2n}$ be a matrix. It is *symplectic* if

$$A^\top J A = J. \quad (2.3)$$

With these definitions, we can then state the following theorem, relating general canonical transformations to symplectic matrices.

Theorem 2.1.6. Let (M, ω_M) and (N, ω_N) be symplectic manifolds. Let $f : M \rightarrow N$ be a diffeomorphism. f is a canonical transformation if and only if df is a symplectic matrix in some coordinate system.

2.2 Hamiltonian Systems

With these definitions of symplecticity in place, we may now introduce Hamiltonian systems. To make the concepts more concrete, we will also go through two standard examples of the simple harmonic oscillator and the pendulum.

Definition 2.2.1. Let (M, ω) be a symplectic manifold, and let $H \in C^\infty(M, \mathbb{R})^1$. (M, ω, H) is called a *Hamiltonian system*. The function H is called the *Hamiltonian*.

Associated with the Hamiltonian is its vector field.

Definition 2.2.2. Let (M, ω, H) be a Hamiltonian system. The *Hamiltonian vector field* X_H is defined as the unique vector field such that for all vector fields Y on M ,

$$dH(Y) = \omega(X_H, Y). \quad (2.4)$$

Expressed in terms of local coordinates, the Hamiltonian vector field is simply

$$X_H = J \nabla H. \quad (2.5)$$

¹ $C^k(M, N)$ is the set of all C^k functions $F : M \rightarrow N$.

Since $J^{-1} = J^{\top} = -J$, writing the vector field in generalized coordinates yields a much more familiar form,

$$\begin{aligned}\dot{q} &= \frac{\partial H}{\partial p} \\ \dot{p} &= -\frac{\partial H}{\partial q},\end{aligned}\tag{2.6}$$

where the dot represents the derivative with respect to time. They are called *Hamilton's equations*.

Let us consider the following simple examples.

Example 2.2.3. Consider the Hamiltonian of the simple harmonic oscillator

$$H(q, p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2.$$

The Hamiltonian is autonomous. The phase space is in $\mathbb{R}^2$, and Hamilton's equations are

$$\begin{aligned}\dot{q} &= \frac{p}{m} \\ \dot{p} &= -m\omega^2 q.\end{aligned}$$

Taking one time derivative of $\dot{q}$ and substituting, we obtain

$$\ddot{q} = -\omega^2 q.$$

Direct integration provides us with the solution

$$\begin{aligned}q &= c_0 \cos(\omega t + c_1) \\ p &= -c_0 m \omega \sin(\omega t + c_1),\end{aligned}$$

and we see that all of the trajectories, aside from the fixed point at $(0, 0)$, are periodic, with fixed frequency of ω . □

Example 2.2.4. As a slightly more nontrivial example, let us consider the Hamiltonian of the pendulum of mass m and arm length l

$$H(q, p) = \frac{p^2}{2ml^2} - mgl \cos q.$$

The Hamiltonian is, again, autonomous, and the system has the phase space of $S^1 \times \mathbb{R}$, i.e. the configuration space is the circle, with the assumption that the arm length is fixed.

Hamilton's equations are

$$\begin{aligned}\dot{q} &= \frac{p}{ml^2} \\ \dot{p} &= -mgl \sin q.\end{aligned}$$

Its fixed points are $(n\pi, 0)$, for $n = 0, \pm 1$.

Following a similar approach as before, we obtain the differential equation

$$\ddot{q} = -\frac{g}{l} \sin q,$$

which, unfortunately, has no solution in terms of elementary functions². However, if we assume that q is small and that $\sin q \approx q$, the system reduces to the case of the simple harmonic oscillator, whose trajectories we know to be periodic. $\square$

What we have described are two simple Hamiltonian systems. Examples of more complex systems are the n -body problem and the electromagnetic forces.

Note that in these examples, there is no explicit dependence on the time variable; thus these systems are all autonomous. Throughout this paper, we will only investigate the case of autonomous systems, particularly due to their well-behavedness, stated in the following proposition.

Proposition 2.2.5. *Let H be a Hamiltonian function, whose corresponding system is autonomous. Then, for a fixed trajectory, $\dot{H} = 0$.*

² The solution is expressed in terms of Jacobi elliptic functions.

In the physical context, autonomy of the Hamiltonian means that the total energy of the system remains unchanged when traversing along a fixed trajectory, i.e. the system obeys the conservation of energy.

We now make a connection between the Hamiltonian and the symplectic form.

Theorem 2.2.6. *Let (M, ω, H) be a Hamiltonian system with X_H the Hamiltonian vector field. Then the flow of X_H preserves ω .*

This is an immediate consequence of Theorem 2.1.6.

2.3 Action-Angle Coordinates

While the behavior of a system is explicitly determined when we obtain the solution trajectories, there exists an alternate way in which similar results may be obtained. This is done via a coordinate transformation to the so-called action-angle coordinates.

When cast in these coordinates, the behavior of the Hamiltonian system becomes very clear. Thus, it will be key to the development of the theory in later chapters. We therefore take the time to establish its existence and construct this coordinate transformation carefully.

Definition 2.3.1. Let H be a Hamiltonian function with a corresponding $2n$ -dimensional system. The system is in *action-angle* form if there exists a coordinate transformation $(q, p) \mapsto (\theta, I)$ such that, when written in terms of (θ, I) , H does not depend on θ , i.e. $H(q, p) \mapsto H(I)$.

θ is called the *angle variable*, while I is the *action variable*.

The new coordinates (θ, I) can be thought of as locally on $\mathbb{T}^n \times \mathbb{R}^n$.

Suppose we are able to find such a coordinate transformation. Then, in these coordinates, the Hamiltonian is written as $H(I)$, and Hamilton's equations become

Figure 2.1: In action-angle transformations, $(q, p) \mapsto (\theta, I)$, which can be thought of as mapping circles (left) to lines (right), with the restriction that in (θ, I) coordinates, I is constant.

extremely simple

$$\begin{aligned}\dot{\theta} &= \frac{\partial H}{\partial I} = \nabla H \\ \dot{I} &= -\frac{\partial H}{\partial \theta} = 0.\end{aligned}\tag{2.7}$$

They can be solved very easily

$$\begin{aligned}\theta(t) &= t\nabla H + \theta_0 \\ I(t) &= I_0.\end{aligned}$$

In other words, if $n = 1$, the transformation can be thought of as mapping circles to lines (Fig. 2.1). In addition, from the special lack of dependence of H on θ , $\dot{\theta}$ is usually called the *frequency vector*, or $\omega(I)$.

To construct these coordinates from (q, p) , we first define the i^{th} coordinate of the action variable to be

$$I_i = \frac{1}{2\pi} \oint p_i dq_i,\tag{2.8}$$

where the integration is performed along a fixed trajectory of the system, i.e. a path of constant energy by Proposition 2.2.5.

In order to construct the transformation $(q, p) \mapsto (\theta, I)$, we utilize what is called the *generating function of type F_2* , which acts as a bridge between the old and the new coordinates. These are derived from Hamilton's principle, which produces four basic types of generating functions, all of which contain half of an even mixture of old and new coordinates. Ones of type F_2 are of special interest, since they have the form

$$S = S(q, \hat{p}), \quad (2.9)$$

where $(\hat{q}, \hat{p})$ is the set of new coordinates. They have the special attribute of satisfying

$$\hat{q} = \frac{\partial S}{\partial \hat{p}} \quad (2.10)$$

$$p = \frac{\partial S}{\partial q}. \quad (2.11)$$

For more details, we refer to Goldstein ([Gol02]).

Example 2.3.2. A simple example of a generating function that does not necessarily produce action-angle coordinates is

$$S(q, \hat{p}) = q^\top \hat{p}. \quad (2.12)$$

Its transformation equations are, naturally

$$\hat{q} = q$$

$$p = \hat{p}.$$

Thus S is called the *generating function for the identity transformation*. □

This transformation will be useful when we consider perturbation and KAM theories.

To construct generating functions for transformation to action-angle coordinates,

however, we notice that, together, Eq. (2.8) and Eq. (2.11) define a partial differential equation that the generating function satisfies. Therefore, to obtain S , we simply integrate it.

We need to be careful, however, and note that S is a function of q and I , thus we must make the appropriate substitutions. In the context of action-angle coordinates, this means that we need to obtain I . This is done by rewriting the Hamiltonian such that $p = p(q, E)$, where E is the energy of the system, which is fixed along each trajectory, then performing the integration over an entire period.

To be more precise, we will go through an example involving the simple harmonic oscillator.

Example 2.3.3. Progressing along with the simple harmonic oscillator, we have, at constant energy,

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2,$$

or

$$p = \sqrt{2mE - m^2\omega^2 q^2},$$

where, for simplicity, we have ignored the negative case. Thus, the action variable is

$$I = \frac{1}{2\pi} \oint \sqrt{2mE - m^2\omega^2 q^2} dq.$$

Utilizing the substitution

$$q = \sqrt{\frac{2E}{m\omega^2}} \sin u,$$

we get

$$\begin{aligned} I &= \frac{\sqrt{E}}{\pi\omega} \oint \sqrt{E - E \sin^2 u} \cos u du \\ &= \frac{E}{\pi\omega} \oint \cos^2 u du \\ &= \frac{E}{\omega}, \end{aligned}$$

where, due to the substitution and the fact that we are working in $\mathbb{R}^2$, the integral becomes a standard integral, with limits of integration of 0 and 2π .

Noting that the generating function satisfies Eq. (2.11), we have

$$\begin{aligned}\frac{\partial S}{\partial q} &= \sqrt{2mE - m^2\omega^2 q^2} \\ &= \sqrt{2m\omega I - m^2\omega^2 q^2}.\end{aligned}$$

We integrate to obtain

$$S = \int \sqrt{2m\omega I - m^2\omega^2 q^2} dq + f(I),$$

where $f(I)$ is the constant of integration.

In addition, we know that it also satisfies Eq. (2.10), so we partially differentiate with respect to I

$$\begin{aligned}\frac{\partial S}{\partial I} &= m\omega \int \frac{1}{\sqrt{2m\omega I - m^2\omega^2 q^2}} dq + f'(I) \\ &= \sin^{-1} \left(\sqrt{\frac{m\omega}{2I}} q \right) + \theta_0 + f'(I),\end{aligned}$$

which is exactly the angle variable θ . We then obtain

$$q = \sqrt{\frac{2I}{m\omega}} \sin(\theta - \theta_0 - f'(I)).$$

The coordinate change for p may then be calculated

$$\begin{aligned}p^2 &= 2m\omega I - m^2\omega^2 q^2 \\ &= 2m\omega I (1 - \sin^2(\theta - \theta_0 - f'(I))) \\ &= 2m\omega I \cos^2(\theta - \theta_0 - f'(I)).\end{aligned}$$

The Hamiltonian, written in action-angle coordinates, is then

$$H(\theta, I) = \omega I,$$

and we see that the dependence on the angle coordinate has disappeared entirely, as desired. □

Although the behavior of the pendulum is more interesting than the simple harmonic oscillator and will be a point of focus later in the discussion, this process is not as illuminating when applied to the pendulum due to its intricacy and usage of Jacobi elliptic functions. We thus leave it to the curious reader to explore. It is also illustrated by Brizard ([Bri13]).

We can ask a question that naturally follows: given a Hamiltonian system, what are the conditions for the existence of an action-angle transformation? The answer lies in Liouville integrability.

Definition 2.3.4. Let (M, ω, H) be a $2n$ -dimensional Hamiltonian system. A function $F : M \rightarrow \mathbb{R}$ is an *integral of motion* if it is constant along individual trajectories, i.e. for all solution trajectories $\gamma : [a, b] \rightarrow M$ and for all $t \in [a, b]$,

$$F(\gamma(t)) = F(\gamma(a))$$

For example, all autonomous Hamiltonians are integrals of motion of their corresponding systems by Proposition 2.2.5. It is an easy exercise to verify for the simple harmonic oscillator, which we leave to the reader.

Definition 2.3.5. A $2n$ -dimensional Hamiltonian system is *Liouville integrable* if it has $2n$ integrals of motion.

In particular, in the setting of Hamiltonian systems, Liouville integrability guarantees the existence of a neighborhood in which such a coordinate transformation to action-angle coordinates exists ([Arn78]). Thus, all autonomous, degree-one (i.e. 2-dimensional) systems can be transformed into action-angle coordinates. However, the transformation may not be defined globally, e.g. the pendulum at the separatrix.

Before moving on, we note that the action-angle transformation is a canonical transformation. Thus, all generating functions (of type F_2) produce canonical transformations.

2.4 Lagrangian Systems

Historically, the construction of Hamiltonian systems is done through the reformulation of Lagrangian mechanics. Although the resulting definition of Hamiltonian systems is equivalent to ours, symplecticity appears as a coincidental consequence rather than an attribute built-in to the definition.

For reasons that will become apparent later, we briefly detract and define Lagrangian systems, illustrate Hamilton's principle via calculus of variations, and establish the link between Hamiltonian and Lagrangian systems.

We shall mainly follow Maruskin ([Mar12]) for the definitions and theorems in this section.

Definition 2.4.1. Let Q be an n -dimensional manifold. A *Lagrangian* function is a function $L : TQ \rightarrow \mathbb{R}$. A *Lagrangian system* is a pair (Q, L) .

Rather than using the generalized position and momentum (q, p) , it is conventional to use $(q, \dot{q})$ instead, where $q \in Q$. Q is called the *configuration space*.

Lagrangian mechanics is derived from a variational principle. Before stating the principle, we require some prerequisite definitions.

Definition 2.4.2. Let Q be an n -dimensional configuration space. Let $q_1, q_2 \in Q$ and $[a, b] \subseteq \mathbb{R}$. We define the *path space* to be the set of C^2 curves (paths) with endpoints of q_1 and q_2 , or

$$\Omega(q_1, q_2, [a, b]) = \{ \gamma \in C^2([a, b], Q) : \gamma(a) = q_1 \wedge \gamma(b) = q_2 \}. \quad (2.13)$$

Definition 2.4.3. A *functional* on an n -dimensional configuration space is a function of curves $S : \Omega(q_1, q_2, [a, b]) \rightarrow \mathbb{R}$. In particular, given a Lagrangian L , the functional defined by

$$S(\gamma) = \int_a^b L(\gamma(t), \dot{\gamma}(t)) dt \quad (2.14)$$

is called the *action functional*, *action integral*, or simply *action*.

Due to the variational nature of the principle from which Lagrangian mechanics is derived, we delve briefly into calculus of variations.

Definition 2.4.4. Let $\gamma : [a, b] \rightarrow Q$. Let $\theta : [-\varepsilon, \varepsilon] \times [a, b] \rightarrow Q$ be C^2 and such that

- For all $t \in [a, b]$, $\theta(0, t) = \gamma(t)$, and
- For all $s \in [-\varepsilon, \varepsilon]$, $\theta(s, a) = \gamma(a)$ and $\theta(s, b) = \gamma(b)$.

Then θ is called a *variation* of γ .

Given this, the *virtual displacement*, or *infinitesimal variation*, associated with θ is defined as

$$\delta\gamma(t) = \left. \frac{\partial \theta(s, t)}{\partial s} \right|_{s=0} \in T_{\gamma(t)}Q. \quad (2.15)$$

In a classical abuse of notation, if $\gamma : [a, b] \rightarrow Q$ is a curve, we will assume³ that there exists a global change of coordinates to put γ such that $t \mapsto (q^1(t), \dots, q^n(t))$. In addition, depending on the context, we will refer q^i as either the coordinate functions of γ or the coordinates themselves. Similarly for $\dot{\gamma}$, $\delta\gamma$, and $\delta\dot{\gamma}$.

Definition 2.4.5. Let $\gamma : [a, b] \rightarrow Q$ and $\theta : [-\varepsilon, \varepsilon] \times [a, b] \rightarrow Q$ be a variation of γ . The *canonical lift* of γ to the tangent bundle TQ is $\hat{\gamma} : [a, b] \rightarrow TQ$ such that $\hat{\gamma}(t) = (\gamma(t), \dot{\gamma}(t))$. Similarly, the *canonical lift* of θ is $\hat{\theta} : [-\varepsilon, \varepsilon] \times [a, b] \rightarrow TQ$ with $\hat{\theta}(s, t) = \left(\theta(s, t), \frac{\partial \theta(s, t)}{\partial t} \right)$.

³ This is most likely an incorrect assumption in general, due to the lack of universal coordinate patches.

Given $\hat{\gamma}$ and a corresponding variation $\hat{\theta}$, the virtual displacement is then, using Einstein notation,

$$\begin{aligned}\delta\hat{\gamma} &= \left. \frac{\partial \hat{\theta}(s, t)}{\partial s} \right|_{s=0} \\ &= \delta q^i \frac{\partial}{\partial q_i} + \delta \dot{q}^i \frac{\partial}{\partial \dot{q}^i}.\end{aligned}$$

Definition 2.4.6. Let $\gamma : [a, b] \rightarrow Q$ and let $\theta : [-\varepsilon, \varepsilon] \times [a, b] \rightarrow Q$ be a variation of γ . Let $f : TQ \rightarrow \mathbb{R}$. The *variation of f with respect to θ* is defined as

$$\delta f = \delta\hat{\gamma}(f), \quad (2.16)$$

which is, in local coordinates,

$$\delta\hat{\gamma}(f) = \frac{\partial f}{\partial q^i} \delta q^i + \frac{\partial f}{\partial \dot{q}^i} \delta \dot{q}^i. \quad (2.17)$$

The variational principle can now be stated as follows.

Definition 2.4.7 (Hamilton's Principle). Let (Q, L) be a Lagrangian system. Let $\gamma : [a, b] \rightarrow Q$ with $\gamma(a) = q_1$ and $\gamma(b) = q_2$. If the curve γ produces an extremal value for the action integral with respect to all variations of γ , γ is said to satisfy *Hamilton's principle*, or *principle of least action*.

The fundamental lemma on which calculus of variations is built can now be stated.

Lemma 2.4.8 (Fundamental Lemma of Calculus of Variations). *Let $f : [a, b] \rightarrow \mathbb{R}$ be a continuous function such that for all continuous $h : [a, b] \rightarrow \mathbb{R}$ with $h(a) = h(b) = 0$, it satisfies*

$$\int_a^b f(t)h(t) dt = 0. \quad (2.18)$$

Then $f(t) = 0$ for all $t \in [a, b]$.

With these ingredients in place, we can state and derive the equations of motion defining Lagrangian mechanics from Hamilton's principle.

Theorem 2.4.9 (Euler-Lagrange Equations). *Let (Q, L) be a Lagrangian system. Fix $q_1, q_2 \in Q$ and $[a, b] \in \mathbb{R}$. A curve $\gamma: [a, b] \rightarrow Q$ is extremal for the action integral if and only if it satisfies*

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0. \quad (2.19)$$

Note that Eq. (2.19) is actually a set of equations, one for each coordinate.

Proof. Let $\theta: [-\varepsilon, \varepsilon] \times [a, b] \rightarrow Q$ be a variation of γ . Then, for each fixed $s \in [-\varepsilon, \varepsilon]$ with the corresponding curve γ_s , we have the action integral

$$S(\gamma_s) = \int_a^b L(\gamma_s, \dot{\gamma}_s) dt.$$

Differentiating with respect to s , we obtain the variation of S with respect to θ , or, using the form in local coordinates, we have

$$\begin{aligned} \delta S(\gamma, \theta) &= \left. \frac{dS(\gamma_s)}{ds} \right|_{s=0} \\ &= \int_a^b \delta \hat{\gamma}(L) dt \\ &= \int_a^b \frac{\partial L}{\partial \dot{q}^i} \delta \dot{q}^i + \frac{\partial L}{\partial q^i} \delta q^i dt. \end{aligned}$$

Integrating the second term by parts, we get

$$\int_a^b \frac{\partial L}{\partial \dot{q}^i} \delta \dot{q}^i dt = \left. \frac{\partial L}{\partial \dot{q}^i} \delta q^i \right|_a^b - \int_a^b \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} \delta q^i dt.$$

By the definition of variations, the first term evaluates to 0, and we obtain

$$\delta S(\gamma, \theta) = \int_a^b \left(\frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} \right) \delta q^i dt.$$

By direct application of Lemma 2.4.8 and the fact that the choice of the variation θ was arbitrary, we immediately obtain Eq. (2.19). □

Here, Eq. (2.19) is called the set of Euler-Lagrange Equations.

Although this proof may appear slightly out of place in comparison to the rest of the paper, we took the effort to establish it, as a discrete analog will be used later.

Finally, we connect between Lagrangian systems and Hamiltonian systems with the fiber derivative.

Definition 2.4.10. Let (Q, L) be a Lagrangian system. The *fiber derivative of L* is a function $\mathbb{F}L : TQ \rightarrow T^*Q$ that maps from the tangent bundle to the cotangent bundle. In local coordinates, it is

$$(q^i, \dot{q}^j) \mapsto \left(q^i, \frac{\partial L}{\partial \dot{q}^j} \right),$$

where, in the second coordinate in the cotangent bundle, we define the quantity

$$p_j = \frac{\partial L}{\partial \dot{q}^j} \tag{2.20}$$

to be the *generalized momentum* corresponding to the coordinate q^j .

The exact relation between Lagrangian and Hamiltonian systems can then be quantified.

Definition 2.4.11. Let (Q, L) be a Lagrangian system. If the fiber derivative $\mathbb{F}L$ is a diffeomorphism, then the corresponding Hamiltonian $H : T^*Q \rightarrow \mathbb{R}$ is defined as

$$H(q, p) = \langle p, \dot{q} \rangle - L(q, \dot{q}). \tag{2.21}$$

In particular, this transformation is called the *Legendre transform*.

Here, $\langle p, \dot{q} \rangle$ is the standard inner product between the two coordinates. Thus we have obtained an alternate, yet equivalent, definition for Hamiltonian systems.

We now go through the example of the simple harmonic oscillator and the pendulum. To construct the Lagrangian, we make use of the definition of the Lagrangian

in classical mechanics, $L = K - U$, the kinetic minus the potential energy. Rather than going through the intricate details of constructing the individual components of the system then applying the laws of Newtonian mechanics, we leave it as an exercise.

Example 2.4.12. In the simple harmonic oscillator, we have the Lagrangian

$$L(q, \dot{q}) = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2 q^2.$$

The generalized momentum is

$$p = m\dot{q}.$$

Noting that rather than substituting the generalized momentum into the inner product directly, we want to eliminate $\dot{q}$ instead due to the lack of explicit dependence of the Hamiltonian on $\dot{q}$, we obtain

$$\begin{aligned} H(q, p) &= \left\langle p, \frac{p}{m} \right\rangle - \frac{1}{2}m\dot{q}^2 + \frac{1}{2}m\omega^2 q^2 \\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 \end{aligned}$$

as the Hamiltonian, which matches our initial example of the simple harmonic oscillator. □

Example 2.4.13. For the pendulum, the Lagrangian is

$$L(q, \dot{q}) = \frac{1}{2}ml^2\dot{q}^2 + mgl \cos q.$$

Following the same procedure, we obtain the generalized momentum,

$$p = ml^2\dot{q},$$

and the corresponding Hamiltonian,

$$\begin{aligned} H(q, p) &= \left\langle p, \frac{p}{ml^2} \right\rangle - \frac{1}{2}ml^2\dot{q}^2 - mgl \cos q \\ &= \frac{p^2}{2ml^2} - mgl \cos q, \end{aligned}$$

which, again, matches the example before. □

It is interesting to note that, had we gone through the construction of the Lagrangians explicitly, we would have encountered the momenta to be exactly what we derived. Here, however, we observe that the correct forms for linear and angular momenta naturally appear as a consequence of the shift from the Lagrangian to the Hamiltonian framework.

At last, we now have the relationship between Lagrangian and Hamiltonian systems. Thus, whatever result we obtain from one framework can be directly translated to the other. It is a matter of convention and convenience that we choose to work with one over the other.

CHAPTER 3

KAM THEORY

In this chapter, we attempt to motivate and explain the progression of the initial development of the subject of KAM theory through perturbation theory. We then state the main theorem and describe its proof in an illustrative manner to preserve clarity and avoid confusion.

Although its derivation can be accomplished without using action-angle coordinates ([dGJV05]), we use these coordinates due to the simplicity of the Hamiltonian in this form and the existence of a canonical transformation to place the result in the original coordinates.

3.1 Perturbation Theory

KAM theory has its roots in classical perturbation theory. Thus, it is natural that we first touch on its basics and motivate the development of KAM theory through the problems of small divisors.

In perturbation theory, given a Liouville integrable Hamiltonian, we are concerned with studying the behavior of the Hamiltonian under small, real-analytic perturbations. In particular, the resulting Hamiltonian may have the form

$$H(\theta, I) = \mathcal{H}(I) + \varepsilon \mathcal{H}_{\text{pert}}(\theta, I). \quad (3.1)$$

Due to Liouville integrability of the initial Hamiltonian $\mathcal{H}$, we have dropped the dependence on θ . However, the perturbation term $\mathcal{H}_{\text{pert}}$ and the resulting perturbed Hamiltonian H may not necessarily be integrable; thus, they may still retain the dependence on the angle coordinate. The behavior we are most often concerned with is

the preservation of invariant tori. That is, given a fixed I^* , we are concerned about whether the frequency vector there, $\omega(I^*)$, remains constant after tacking on the perturbation term.

The underlying idea is that there exists some near-identity canonical transformation such that, for small enough ε , the perturbed Hamiltonian takes on the action-angle form under the transformation, possibly with new coordinates $(\hat{\theta}, \hat{I})$. Namely, our goal is to find a generating function $S(\theta, \hat{I})$ such that

$$\begin{aligned} H\left(\theta, \frac{\partial S}{\partial \theta}\right) &= \mathcal{H}\left(\frac{\partial S}{\partial \theta}\right) + \varepsilon \mathcal{H}_{\text{pert}}\left(\theta, \frac{\partial S}{\partial \theta}\right) \\ &= \hat{\mathcal{H}}(\hat{I}) \end{aligned}$$

with

$$\left. \frac{\partial \mathcal{H}}{\partial I} \right|_{I^*} = \left. \frac{\partial \hat{\mathcal{H}}}{\partial \hat{I}} \right|_{\hat{I}^*}.$$

Without loss of generality, since we can simply use a canonical transformation to shift the origin to I^* , we will assume $I^* = 0$.

Naively, since we want a near-identity transformation, perhaps the generating function is near-identity as well, and we are looking for a generating function that looks like

$$S(\theta, \hat{I}) = \theta^\top \hat{I} + \varepsilon \mathcal{S}(\theta, \hat{I}), \quad (3.2)$$

because the canonical transformation then takes the form

$$\begin{aligned} I &= \frac{\partial S}{\partial \theta} \\ &= \hat{I} + \varepsilon \frac{\partial \mathcal{S}}{\partial \theta} \\ \hat{\theta} &= \frac{\partial S}{\partial \hat{I}} \\ &= \theta + \varepsilon \frac{\partial \mathcal{S}}{\partial \hat{I}}, \end{aligned} \quad (3.3)$$

where the hats denote the (possibly) new action-angle coordinates.

Substituting in to the perturbed Hamiltonian (Eq. (3.1)), we obtain

$$H(\theta, I) = \mathcal{H} \left(\hat{I} + \varepsilon \frac{\partial \mathcal{S}}{\partial \theta} \right) + \varepsilon \mathcal{H}_{\text{pert}} \left(\theta, \hat{I} + \varepsilon \frac{\partial \mathcal{S}}{\partial \theta} \right).$$

Taylor expanding both terms around $\varepsilon = 0$, truncating at the first order, and recalling the definition of the frequency vector, it becomes

$$\mathcal{H}(\hat{I}) + \varepsilon \omega(\hat{I})^\top \frac{\partial \mathcal{S}}{\partial \theta} + \varepsilon \mathcal{H}_{\text{pert}}(\theta, \hat{I}).$$

Since we want it to be in action-angle form, we see that we must have the terms containing θ summing to zero, i.e.

$$\omega(\hat{I})^\top \frac{\partial \mathcal{S}}{\partial \theta} + \mathcal{H}_{\text{pert}}(\theta, \hat{I}) = 0. \quad (3.4)$$

Using the periodicity about θ , we may rewrite both the perturbation term $\mathcal{H}_{\text{pert}}$ and the generating function $\mathcal{S}$ as Fourier series

$$\begin{aligned} \mathcal{H}_{\text{pert}}(\theta, \hat{I}) &= \sum_{k \in \mathbb{Z}^d \setminus \{0\}} c_k(\hat{I}) e^{2\pi i k^\top \theta} \\ \mathcal{S}(\theta, \hat{I}) &= \sum_{k \in \mathbb{Z}^d \setminus \{0\}} d_k(\hat{I}) e^{2\pi i k^\top \theta}. \end{aligned} \quad (3.5)$$

Note that the Fourier coefficients are still possibly dependent on $\hat{I}$. In addition, the summation is over $\mathbb{Z}^d$, where $0 \leq d \leq n$. Rather than using the dimension of the configuration manifold n , we use d instead, to denote that the tori may have dimensions less than n .

Finally, substituting them in to Eq. (3.4) produces

$$2\pi i \omega(\hat{I})^\top \sum_{k \in \mathbb{Z}^d \setminus \{0\}} k d_k(\hat{I}) e^{i2\pi k^\top \theta} + \sum_{k \in \mathbb{Z}^d \setminus \{0\}} c_k(\hat{I}) e^{i2\pi k^\top \theta} = 0.$$

Comparing term-by-term, we obtain the relation

$$2\pi i k^\top \omega(\hat{I}) d_k(\hat{I}) + c_k(\hat{I}) = 0,$$

or, since we were originally after the generating function itself,

$$d_k(\hat{I}) = -\frac{1}{2\pi i k^\top \omega(\hat{I})} c_k(\hat{I}). \quad (3.6)$$

From this derivation, we see that $d_k(\hat{I})$ exists only when $\omega(\hat{I})^\top k \neq 0$. However, this is clearly not satisfied when $\omega(\hat{I})$ is rationally dependent, or when k is such that the inner product is linearly dependent. In the past, those who worked with perturbation theory usually applied arguments specific to the fields they worked in to establish convergence of the Fourier series. In the most elementary form, they amounted to comparing the cardinality of the rational and irrational numbers. However, problems of this type, called the *small divisor problems*, remained largely unsolved in general until their partial solution by KAM theory.

Slightly digressing, one may wonder why ω was chosen to show the preservation of a torus. It is a theorem in dynamics that an irrational flow on a torus approximates the torus itself arbitrarily well. Thus, all that is needed to prove the KAM theorem is that the quantity ω remains constant under small perturbations.

3.2 Kolmogorov's Theorem

In this section, we will state the KAM theorem by Kolmogorov, using normal forms, as well as the conditions for the theorem to hold. Rather than a detailed proof for this formulation of the theorem, however, we will illustrate an equivalent procedure immediately following where we left off in the previous section of classical perturbation theory, detailed by Wayne ([Way08]).

The original theorem and scheme for the construction of a canonical transformation was first proposed and described in detail by Kolmogorov in 1954, and then proven by Arnold and Moser, in 1963 and 1962, respectively. In the statement of the classical theorem, two concepts are required to overcome the problems relating to convergence.

The first is the usage of a Diophantine condition, and the second the application of a Newton's method.

In Eq. (3.6), while one can certainly make use of the fact that there are many more irrational than rational numbers, this only accounts for one facet of the problem. More specifically, the term $\omega(\hat{I})^\top k$ may become arbitrarily small, dwarfing the Fourier coefficients $c_k(\hat{I})$ ([Poi99]). In such a scenario, the sum may become unbounded as well. One can view this problem as approximating rationals by irrationals. Thus, in general, this series diverges.

We seek a condition in which the resulting set of numbers is sufficiently isolated from rationals. This condition is called Diophantine.

Definition 3.2.1. $\omega_i \in \mathbb{R}$ is said to satisfy the *Diophantine condition (of type (K, ν))* if, for $K > 0$ and $\nu \geq 1$, and for all $\frac{r}{s} \in \mathbb{Q}$,

$$\left| \omega_i - \frac{r}{s} \right| > \frac{K}{|s|^{1+\nu}}. \quad (3.7)$$

We also say that ω_i is *Diophantine*.

As this definition is for $\mathbb{R}$ only, we require a similar definition, but for $\mathbb{R}^d$.

Definition 3.2.2. Given $K > 0$ and $\nu > 0$, we say that $\omega \in \mathbb{R}^d$ satisfies the *strong nonresonance condition (of type (K, ν))*, or the *Siegel's Diophantine condition*, if, for all $k \in \mathbb{Z}^d$,

$$\left| k^\top \omega \right| \geq \frac{K}{\|k\|_1^\nu}, \quad (3.8)$$

where $\|\cdot\|_1$ is the 1-norm.

In addition, in the classical statement of the theorem, we need to define the Kolmogorov normal form.

Definition 3.2.3. Let $H(\theta, I)$ be a Hamiltonian written in the form

$$H(\theta, I) = c + \omega^\top I + \frac{1}{2} I^\top M(\theta, I) I, \quad (3.9)$$

where c is constant, ω satisfies the strong nonresonance condition, and $M(\theta, I)$ is a real, symmetric, d -dimensional matrix. Then $H(\theta, I)$ is said to be in the *Kolmogorov normal form*.

It is called *nondegenerate* if both the Hessian $\frac{\partial^2 M}{\partial I^2}$ and the angular average

$$\overline{M}_0 = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} M(\theta, 0) d\theta \quad (3.10)$$

are invertible.

In Kolmogorov's original paper in 1954 ([Kol54]), the normal form is stated slightly differently, although equivalently, as

$$H(\theta, I) = E + \omega^\top I + Q(\theta, I),$$

with E constant, and $Q(\theta, I)$ and $\frac{\partial Q}{\partial I}$ vanish at $I = 0$.

Still assuming that the point of interest is at $I = 0$, we can now state the main theorem.

Theorem 3.2.4 (KAM). *Let*

$$\mathcal{H}(\theta, I) = c + \omega^\top I + \frac{1}{2} I^\top M(\theta, I) I$$

be a nondegenerate Kolmogorov normal form such that $M(\theta, I)$ is analytic with respect to both θ and I , and ω satisfies the strong nonresonance condition. Let

$$H(\theta, I) = \mathcal{H}(\theta, I) + \varepsilon \mathcal{H}_{\text{pert}}(\theta, I),$$

with $\mathcal{H}_{\text{pert}}(\theta, I)$ a real-analytic Hamiltonian in a neighborhood of

$\{(\theta, I) : \theta \in \mathbb{T}^d \wedge I = 0\}$. Then there exists an $\varepsilon_0 > 0$ and an analytic canonical

transformation $f : (\hat{\theta}, \hat{I}) \rightarrow (\theta, I)$, close to the identity, such that for all $|\varepsilon| \leq \varepsilon_0$, $H \circ f$ is a Kolmogorov normal form

$$H \circ f(\hat{\theta}, \hat{I}) = d + \omega^\top \hat{I} + \frac{1}{2} \hat{I}^\top N(\hat{\theta}, \hat{I}) \hat{I}.$$

In other words, the frequency vector is preserved under small perturbations. Along with the previous observation of equivalence between the preservation of irrational flows on a torus and the preservation of the torus itself, Theorem 3.2.4 implies that tori remain invariant under small perturbations.

Note that in the assumption of the analyticity of $M(\theta, I)$, there exists a canonical transformation to put the Kolmogorov normal form into action-angle coordinates.

Although there are other equivalent statements of the theorem, we stated it in its classical form with the Kolmogorov normal form due to its beauty and simplicity. In particular, in the Kolmogorov normal form, the torus at $\{(\theta, I) : \theta \in \mathbb{T}^d \wedge I = 0\}$ is preserved under the Hamiltonian flow.

Although we will not plunge into the proof in great detail, we will outline it. However, for illustrative purposes, connection back to perturbation theory, and straightforwardness, we will not proceed along the original sketch of proof outlined in [Kol54]¹. Rather, we will briefly describe the procedure when using the Fourier series constructed in perturbation theory, detailed by Wayne ([Way08]).

Upon plugging Eq. (3.6) into the second of Eq. (3.5), we obtain

$$\mathcal{S}(\theta, \hat{I}) = \frac{i}{2\pi} \sum_{k \in \mathbb{Z}^d \setminus \{0\}} \frac{c_k(\hat{I})}{k^\top \omega(\hat{I})} e^{2\pi i k^\top \theta},$$

and we observe that we need to show convergence of an infinite sum. To do so, we truncate the series at some integer N , and call the partial sum $\mathcal{S}_N(\theta, \hat{I})$

$$\mathcal{S}_N(\theta, \hat{I}) = \frac{i}{2\pi} \sum_{k \in \mathbb{Z}^d \setminus \{0\}, |k| \leq N} \frac{c_k(\hat{I})}{k^\top \omega(\hat{I})} e^{2\pi i k^\top \theta}.$$

¹ We will provide an extremely short sketch of the process in the next chapter.

However, this partial sum does not solve Eq. (3.4). Rather, it solves

$$\omega(\hat{I})^\top \frac{\partial \mathcal{S}_N}{\partial \theta} + \sum_{k \in \mathbb{Z}^d \setminus \{0\}, |k| \leq N} c_k(\hat{I}) e^{2\pi i k^\top \theta} = 0.$$

This implies that we should assign a name to the second summation

$$\mathcal{H}_{\text{pert}_N}(\theta, \hat{I}) = \sum_{k \in \mathbb{Z}^d \setminus \{0\}, |k| \leq N} c_k(\hat{I}) e^{2\pi i k^\top \theta}.$$

Recall that the initial derivation of the small divisor problems, we truncated the Taylor series at the linear term. As it turns out, this additional truncation of the Fourier series still maintains the estimation of linear order.

With this truncation, following the form of the near-identity generating function Eq. (3.2), it can be shown that

$$S_N(\theta, \hat{I}) = \theta^\top \hat{I} + \varepsilon \mathcal{S}_N(\theta, \hat{I})$$

is an analytic generating function in the neighborhood of the origin, which then defines an analytic canonical transformation given by

$$\begin{aligned} \hat{\theta} &= \theta + \frac{\partial \mathcal{S}_N}{\partial \hat{I}} \\ I &= \hat{I} + \frac{\partial \mathcal{S}_N}{\partial \theta}. \end{aligned}$$

Applying this canonical transformation to Eq. (3.1), we obtain a new Hamiltonian $H_N(\hat{\theta}, \hat{I})$. Unless in ideal circumstances, it is highly unlikely that this Hamiltonian is in action-angle form, due to the various approximations we have made. However, the entire construction can be repeated for the new Hamiltonian $H_N(\hat{\theta}, \hat{I})$ to obtain yet another canonical transformation.

If we believe that each coordinate transformation linearly approximates the end result of the action-angle coordinates, we are in place to iteratively apply this construction

à la Newton's method. The sequence of canonical transformations will then converge to the action-angle form.

In fact, a few propositions by Wayne ([Way08]) lead to the result that, for all $\xi > 0$, there exists an $n \in \mathbb{N}$ such that at the n^{th} step of the iteration, there exists a domain based around $I = 0$ with some radius $\delta > 0$ such that the coordinate-transformed Hamiltonian at this step is still analytic in this neighborhood. The Hamiltonian can be written in the form of Eq. (3.1) as well, where the perturbation is, at most, ξ away from the case $\varepsilon = 0$.

There is a crucial portion of the proof we need to tread with care, however. As $\xi \rightarrow 0$, naturally $\delta \rightarrow 0$ as well. In order to maintain the well-definedness of the iteration argument due to the progressively-smaller domains, we need to control the N at which we truncate the Fourier series.

This then virtually concludes the sketch of the proof of Theorem 3.2.4, since it can be shown that as the sequence of canonical transformations is iteratively applied to Eq. (3.1), the integrable term converges to ω at $I = 0$. It is then a simple canonical transformation that demonstrates equivalence of results in Theorem 3.2.4.

As a last note in this chapter, proofs of this type typically only show the preservation of a single torus in the Hamiltonian system, and require analyticity of the perturbed Hamiltonian. There are other proofs in which preservation of Cantor sets of tori is the result ([Arn63a] and [Mos62]), and proofs where analyticity is not required ([Mos62]). In particular, Moser's work was on the case when the perturbation term is C^{333} . More recent results from Herman ([Her83]) have shown that the theorem holds for C^k when $k \geq 3$, but does not for $k < 3$.

CHAPTER 4

PRESERVATION OF PERIODIC TRAJECTORIES

One may question the use of KAM theory in the preservation of periodicity of trajectories when they are constructed via integrators applied to Hamiltonian systems. Although the answer is not immediate, it is given by a theorem that allows us to embed specific types of trajectories, and therefore vector fields, in a Hamiltonian flow.

Given this flow, it can then be shown that the constructed Hamiltonian flow has a Hamiltonian that can be written as a perturbation of the original Hamiltonian from which we produced the discrete trajectory. The problem is then cast in the form in which a KAM-type proof can be used to establish the periodicity of the discrete trajectory in the constructed Hamiltonian.

4.1 Embedding Discrete Trajectories

Our first goal is to establish how discrete trajectories can be embedded in a Hamiltonian flow, in order to develop a KAM-like theorem.

On a cursory glance, one might wonder about the contradictory nature between periodicity of discrete trajectories and the requirement of the strong nonresonance condition by Theorem 3.2.4. Recall that, in the classical definition, a trajectory is periodic if it traces and retraces a fixed set of points, i.e. the frequency is resonant. Thus, to directly apply Theorem 3.2.4, we require the trajectory to be nonperiodic, which is clearly not our intention.

Yet another question one may consider is the validity of our goal of periodicity. Since we working in smooth dynamical systems, we naturally want to (smoothly) interpolate the trajectory produced by a numerical integrator. However, if we are to expect

the strong nonresonance condition to hold, the resulting interpolation is most likely not a trajectory in the requirements specified by smooth dynamical systems, due to the interpolation crossing itself.

The answer is to consider the space with an additional time-like dimension, and to embed the trajectories in it.

We will restrict our attention to a particular class of integrators, namely *one-step methods*. They are methods in which the evolution operator is dependent only on one single point, i.e.

$$x_{k+1} = x_k + hf(x_k).$$

Given the vector field f and step size h , we will denote by $\Phi_{h,f}$ the one-step method that produces such a trajectory. We will delve into them in more detail later.

It was stated in a theorem by Moan in 2004 ([Moa04]) and proven in 2005 ([Moa05]) that for all analytic vector fields and one-step methods applied to the vector fields, there exists a modified vector field whose flow interpolates a trajectory traced by the one-step method.

Theorem 4.1.1 (Moan). *Let $\Phi_{h,f}$ be a one-step method for some analytic vector field $f(x)$ in some $D \subseteq \mathbb{C}^n$ and some step size h . Then there exists an analytic vector field*

$$\tilde{f}(x, t, h) = f(x) + \varepsilon r_1(x) + \varepsilon r_2(x, t, h) \tag{4.1}$$

in some $\tilde{D} \subseteq D$, h -periodic in t , whose flow interpolates the trajectory produced by $\Phi_{h,f}$.

In fact, Pronin and Treschev ([PT97]) showed additionally that in such interpolations, if the original map, say, produced by $\Phi_{h,f}$, is symplectic, then $\tilde{f}$ is a Hamiltonian flow.

Note that here, if we translate into the context of Hamiltonian systems, x represents the variables θ and I .

4.2 Preservation of Periodic Trajectories

We are now in place to construct the KAM-like theorem that demonstrates the preservation of periodicity of trajectories by symplectic one-step methods. Like in Theorem 3.2.4, we shall need to define a normal form on which the entire theorem will rely. With this, we can then apply Theorem 4.1.1 and cast the resulting Hamiltonian as a perturbation of the original to obtain the main theorem of this chapter.

Whereas in the classical scheme of KAM theory, the Kolmogorov normal form plays a vital role, the normal form of interest here is called the *Floquet form*

$$H(\theta, x, I, y) = \omega^\top I + \frac{1}{2}(x^\top, y^\top)B(x^\top, y^\top)^\top + H_*(\theta, x, I, y), \quad (4.2)$$

where $B \in \mathbb{C}^{2m \times 2m}$ is a symmetric matrix, H_* is periodic and analytic in all variables, and the Taylor expansion H_* contains no quadratic terms in $(x^\top, y^\top)$ and no linear terms in I .

We have made a few standard assumptions of H , such as analyticity, autonomy, and containing torus of d degrees of freedom with quasiperiodic flow and rationally-independent frequencies $\omega \in \mathbb{R}^r$. In addition, we will assume that the torus is reducible. There then exists a canonical transformation and a splitting of the coordinates into (θ, x, I, y) with $\theta, I \in \mathbb{C}^r$, $x, y \in \mathbb{C}^m$, and $d = r + m$ such that the original Hamiltonian can be put into this Floquet form.

Here, a torus is *reducible* if the linearized flow can be transformed into a first-order linear differential equation with constant coefficients $\dot{z} = Az$. In turn, this implies that all of the quadratic terms are encapsulated by the second quadratic term in the Floquet form, and H_* contains no quadratic terms.

Proceeding in parallel to classical perturbation theory, O’Neale ([O’N09]) showed that the problem of small divisors is slightly different. The denominator is now

$$ik^\top \omega + l^\top \lambda, \quad (4.3)$$

where k corresponds to the r -dimensional index vector on the torus, while l is $2m$ -dimensional index vector for $(x^\top, y^\top)^\top$, and λ is the vector of eigenvalues for $J^{-1}B$.

In order to ensure convergence, we require a Diophantine condition to be satisfied

$$\left| ik^\top \omega + l^\top \lambda \right| \geq \frac{\mu_0}{\|k\|_1^\gamma}, \|l\|_1 \leq 2. \quad (4.4)$$

Under these, our Hamiltonian takes on the form

$$H(\theta, x, I, y) = \omega^\top I + \frac{1}{2}(x^\top, y^\top)B(x^\top, y^\top)^\top + \frac{1}{2}I^\top CI + H_*(\theta, x, I, y). \quad (4.5)$$

C is a constant matrix of nonzero determinant, and H_* is expanded in a power series with some additional requirements on particular individual monomials.

This is the normal form we need to establish the main theorem stated and proven by O'Neale.

Suppose that, for our integrable Hamiltonian system $\mathcal{H}$ with corresponding vector field $X_{\mathcal{H}}$, we are given a one-step method $\Phi_{h, X_{\mathcal{H}}}$ with some step size h . Recall that

$$X_{\mathcal{H}} = J\nabla \mathcal{H}.$$

By Theorem 4.1.1, the modified vector field that interpolates the trajectory is

$$X_H(\theta, x, I, y, \tilde{\theta}, \tilde{I}, h) = X_{\mathcal{H}}(\theta, x, I, y) + \varepsilon r_1(\theta, x, I, y) + \varepsilon r_2(\theta, x, I, y, \tilde{\theta}, \tilde{I}, h),$$

where the variables $\tilde{\theta}$ and $\tilde{I}$ are the new time-like variables. Note that we now switch to the notation of classical perturbation theory, in which the perturbed Hamiltonian is denoted by H , while the original and the perturbation are $\mathcal{H}$ and $\mathcal{H}_{\text{pert}}$, respectively. Here, the perturbed Hamiltonian has the vector field of the modified vector field produced by Theorem 4.1.1.

Defining

$$\begin{aligned} X_{\mathcal{H}_{\text{pert}}} &= J\nabla \mathcal{H}_{\text{pert}} \\ &= \varepsilon(r_1 + r_2), \end{aligned}$$

by analyticity, we can then rewrite the portion containing the new variables $\tilde{\theta}$ and $\tilde{I}$ in the Floquet form

$$\mathcal{H}_{\text{pert}}(\theta, x, I, y, \tilde{\theta}, \tilde{I}, \varepsilon) = \tilde{\omega}\tilde{I} + \varepsilon \tilde{\mathcal{H}}(\theta, x, I, y, \varepsilon).$$

By linearity of derivatives, we obtain

$$\begin{aligned} H &= \mathcal{H} + \mathcal{H}_{\text{pert}} \\ &= \omega^\top I + \tilde{\omega}\tilde{I} + \frac{1}{2}(x^\top, y^\top)B(x^\top, y^\top)^\top + \frac{1}{2}I^\top CI + H_*(\theta, x, I, y) + \varepsilon \tilde{H}(\theta, x, I, y, \varepsilon). \end{aligned} \quad (4.6)$$

With this, we then construct a sequence of canonical transformations via generating functions. After each transformation, the resulting Hamiltonian is then put back into the form in Eq. (4.6). The single remaining condition, the *nondegeneracy condition*, is then stated as the requirements placed upon the relation between the eigenvalues of matrix $J^{-1}B$ prior to and following the first canonical transformation. For details, we refer to [O'N09].

We can now state the main result obtained by O'Neale.

Theorem 4.2.1 (O'Neale). *Let*

$$\mathcal{H}(\theta, x, I, y) = \omega^\top I + \frac{1}{2}(x^\top, y^\top)B(x^\top, y^\top)^\top + \frac{1}{2}I^\top CI + H_*(\theta, x, I, y)$$

be the normal form given in Eq. (4.5) satisfying the conditions of the expansion of H_ , the forms of the matrices B and C , and the Diophantine condition in Eq. (4.4). Moreover, suppose that the nondegeneracy condition is satisfied as well.*

Then there exists a Cantor set such that for all $\tilde{\omega}$ in it, the perturbed Hamiltonian given in Eq. (4.6) has a two-dimensional invariant torus with the frequency vector $(\omega^\top, \tilde{\omega})$ on it.

Since Eq. (4.6) is constructed from a one-step method, the result directly signifies that if a given trajectory in the original Hamiltonian is periodic, the discretized trajectory produced by the one-step method is periodic as well.

Note that the significance of the specific dimension of the torus of two arises from the fact that periodic trajectories are naturally one-dimensional. In utilizing the additional time-like dimension, we naturally extend the one-dimensional torus by the additional dimension, hence the two-dimensional torus. Due to this peculiarity, this theorem appears to yield an immediate generalization to higher-dimensional tori. In fact, this was stated and proven by Jorba and Villaneuva ([JV97]).

CHAPTER 5

CONSTRUCTION OF THE VARIATIONAL INTEGRATOR

Thus far, we have only discussed the theoretical aspects of the existence of discrete trajectories that mirror the periodicity of the original Hamiltonian systems. In this chapter, we illustrate the failure of common numerical integrators to preserve periodicity, and thus the need for symplectic one-step methods. We then explicitly formulate a way of obtaining such integrators via Lagrangian mechanics, more specifically Hamilton's principle. We then demonstrate this integrator in practice by applying it to the simple harmonic oscillator and the pendulum.

5.1 Numerical Integrators

In prior discussions, we have touched on numerical integrators, but have yet to describe them in more detail. We aim to give a brief introduction to two of the commonly-encountered integrators, as well as some concrete evidence why the formulation for symplectic one-step methods is necessary for periodicity, via the simple harmonic oscillator.

The one-step method mentioned in the previous chapter is a subset of common objects seen in numerical analysis: *numerical integrators*, or simply *integrators*. In general, since most systems cannot be integrated explicitly, we need to use another method to obtain the solution trajectories.

For short-term behavior, what has worked well in the past is to utilize the set of differential equations determining the vector field. Rather than treating the vectors to represent infinitesimal evolutions in time, we allow them to take on physically-feasible magnitudes. At the endpoint of the vector, we calculate the corresponding vector that

starts there, and recursively construct a discrete set of points representing the *numerical trajectory*.

Example 5.1.1. An extremely simple example of an integrator that most of us have encountered is *Euler's method*. There, we take the vector field that produces the discrete trajectory to be the vector field of the original continuous system. I.e., in the context of Hamiltonian systems, assuming that (q_0, p_0) is the initial point, points in the trajectory are defined by the relation

$$\begin{pmatrix} q_{k+1} \\ p_{k+1} \end{pmatrix} = \begin{pmatrix} q_k \\ p_k \end{pmatrix} + X_H(q_k, p_k).$$

□

Note that another way of stating the relationship between the new vector field and X_H is that, in Euler's method, it is scaled to be a unit multiple of the original vector field. Thus, the main problem in numerical analysis may be stated as finding the ideal vector field modification such that the resulting set of numerical trajectories is quantitatively or qualitatively (or both) the same as that of the continuous system.

Of course, the modification process may not necessarily depend on the vector field value at one particular point. If it depends on two or more prior points, the method is called a *multi-step method*. In contrast, Euler's method and the more popular *ode45* solver in Matlab are both one-step methods. However, in most explicit examples, we will only consider Euler's method due to its simplicity and its explicit characterization of the undesirable features present in a large portions of classical numerical integrators.

A common observation is that, to attempt to increase accuracy, we may also multiply the vector field by an increasingly smaller scalar value, i.e. decrease the time-step size. While this is true in the limit, the qualitative long-term behavior of the

Figure 5.1: A trajectory produced by Euler's method applied to the simple harmonic oscillator.

resulting intermediate numerical trajectories may not necessarily be comparable to the trajectories from the original system.

Example 5.1.2. Recall that the simple harmonic oscillator has the following Hamilton's equations of motion

$$\begin{aligned}\dot{q} &= \frac{p}{m} \\ \dot{p} &= -m\omega^2 q.\end{aligned}$$

Recall from Example 2.2.3 that every trajectory, aside from the single fixed point, is periodic.

Figure 5.2: Distance between the n th return map and the initial point of the trajectory, as a function of n . The left uses Euler's method, while the right uses *ode45*, applied to the simple harmonic oscillator.

Applying Euler's method, we obtain the recurrence system

$$\begin{aligned} q_{k+1} &= q_k + \frac{hp_k}{m} \\ p_{k+1} &= p_k - hm\omega^2 q_k, \end{aligned}$$

where h is the step size.

Plotting a trajectory with a nonzero starting point (Fig. 5.1) hints that we have lost the periodicity. In particular, if we plot the distance from the initial point to each of the return maps as a function of the number of returns (Fig. 5.2, left), we see that for all $h > 0$, periodicity is no longer present. In fact, the only point to retain its qualitative feature¹ is the origin, which remains a fixed point.

A similar picture may be painted using Matlab's built-in *ode45* (Fig. 5.2, right). $\square$

The destruction of periodic trajectories is not only true for the simple harmonic oscillator and the pendulum, but observable for general systems as well.

¹ This is only considering pointwise. As soon as we take any nonzero neighborhood, this is no longer true.

5.2 Variational Integrators

While we have demonstrated our need for a symplectic one-step method, we have yet to obtain one explicitly. In this section, we follow West ([Wes04]) to obtain the so-called variational integrators, and to see the effect of the application to both the simple harmonic oscillator and the pendulum.

By the results of O’Neale, we know that for all one-step symplectic integrators, the periodicity is preserved, provided that the assumptions are satisfied. West ([Wes04]) showed, in 2004, an intuitive way in which a particular class of symplectic one-step methods may be constructed, via the Lagrangian framework. More specifically, starting from Hamilton’s principle, we derive an analog by following along the proof of Theorem 2.4.9 of constructing the Euler-Lagrange equations (Eq. (2.19)), except in a discrete fashion.

That is, starting from the Lagrangian, we discretize it to be

$$L_d(q_k, q_{k+1}, h) = \int_{t_k}^{t_{k+1}} L(q, \dot{q}) dt.$$

The main reason for this form, as detailed by West ([Wes04]), is to obtain an exact correspondence between continuous and discrete systems. Here, $h = t_{k+1} - t_k$, and we have made the assumption that $\dot{q}$ is a function of q_k and q_{k+1} , e.g. the case of Euler’s method. Then, assuming that the trajectory is a discrete set of points $\{q_i\}_{i=0}^N$, the action integral turns into a finite sum

$$S_d(\{q_k\}_{k=0}^N) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}, h),$$

which, taking variations with q_0 and q_N fixed, gives us

$$\begin{aligned} \delta S_d(\{q_k\}_{k=0}^N) &= \sum_{k=0}^{N-1} \frac{\partial L_d}{\partial q_k}(q_k, q_{k+1}, h) \delta q_k + \frac{\partial L_d}{\partial q_{k+1}}(q_k, q_{k+1}, h) \delta q_{k+1} \\ &= \sum_{k=1}^{N-1} \left(\frac{\partial L_d}{\partial q_k}(q_k, q_{k+1}, h) + \frac{\partial L_d}{\partial q_k}(q_{k-1}, q_k, h) \right) \delta q_k, \end{aligned}$$

where fixing q_0 and q_N implies that $\delta q_0 = \delta q_N = 0$.

Recalling Lemma 2.4.8 and requiring Hamilton's principle to be satisfied yields

$$\frac{\partial L_d}{\partial q_k}(q_k, q_{k+1}, h) + \frac{\partial L_d}{\partial q_k}(q_{k-1}, q_k, h) = 0. \quad (5.1)$$

This is called the *discrete Euler-Lagrange equations*.

The derivation for the discretized Lagrangian, and therefore Eq. (5.1), holds in general for numerical integrators that are dependent on a single prior point, i.e. one-step methods. Unfortunately, dependence on a higher number of points (multi-step methods) does not work out. Although perhaps additional conditions for dependence on k prior points such as C^{k+1} smoothness for parts of the resulting equation that are not overlapped by every term may be used to uniquely determine the equations of motion, it corresponds to no physical analog of Hamilton's principle that we know of.

From the discrete Euler-Lagrange equations (Eq. (5.1)), we can then deduce the recurrence relations governing the discrete evolution of individual trajectories by utilizing the definition for generalized momenta Eq. (2.20),

$$\begin{aligned} p_k &= -\frac{\partial L_d}{\partial q_k}(q_k, q_{k+1}, h) \\ &= \frac{\partial L_d}{\partial q_k}(q_{k-1}, q_k, h), \end{aligned}$$

or, reindexing,

$$\begin{aligned} p_k &= -\frac{\partial L_d}{\partial q_k}(q_k, q_{k+1}, h) \\ p_{k+1} &= \frac{\partial L_d}{\partial q_{k+1}}(q_k, q_{k+1}, h). \end{aligned} \quad (5.2)$$

The integrators satisfying this relation are called *variational integrators*. It is important to note the distinction between the integrator we initially used for the Lagrangian and the integrator that we derived. In general, the one for the Lagrangian will not necessarily be variational.

A short calculation in West proves the following theorem.

Theorem 5.2.1 (West). *The equations of motion determined by variational integrators define a symplectic map, in both the Lagrangian and the Hamiltonian framework.*

Pooling this result and one from O’Neale, we have an immediate corollary that the discretized trajectories obtained from variational integrators have their periodicities preserved, for frequencies satisfying the Diophantine condition (Eq. (4.4)).

Corollary 5.2.2. *Let $\mathcal{H}$ satisfy the assumptions of Theorem 4.2.1 with frequency vector ω , and let $\Phi_{h,X,\mathcal{H}}$ be a variational integrator. Then, for frequencies $(\omega^\top, \tilde{\omega})$ satisfying Eq. (4.4), the perturbed Hamiltonian in Eq. (4.6) corresponding to $\Phi_{h,X,\mathcal{H}}$ has a two-dimensional invariant torus with frequency vector $(\omega^\top, \tilde{\omega})$.*

Example 5.2.3. Let us derive a variational integrator for the simple harmonic oscillator, using Euler’s method and the one-point quadrature at the left endpoint.

The Lagrangian is

$$L(q, \dot{q}) = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2 q^2,$$

which discretizes to

$$\begin{aligned} L_d(q_k, q_{k+1}, h) &= hL\left(q_k, \frac{q_{k+1} - q_k}{h}\right) \\ &= \frac{m(q_{k+1} - q_k)^2}{2h} - \frac{hm\omega^2 q_k^2}{2}. \end{aligned}$$

Its partial derivatives are

$$\begin{aligned} p_k &= \frac{m(q_{k+1} - q_k)}{h} + hm\omega^2 q_k \\ p_{k+1} &= \frac{m(q_{k+1} - q_k)}{h}, \end{aligned}$$

Figure 5.3: Distance between the n th return map and the initial point of the trajectory, as a function of n . This uses the variational integrator applied to the simple harmonic oscillator. Notice that the distances are measured on the scale of $1e-5$.

or, rewriting it slightly,

$$q_{k+1} = q_k + \frac{hp_{k+1}}{m}$$

$$p_{k+1} = p_k - hm\omega^2 q_k,$$

which looks incredibly similar in form to the system obtained by directly discretizing Hamilton's equations via Euler's method.

By O'Neale, the discrete periodic trajectory now lies on the torus $\mathbb{T}^2$, having an extra time-like dimension. Since it is difficult to paint the picture of periodicity there, we utilize return maps instead (Fig. 5.3), in a similar fashion as the illustrations for Euler's method and *ode45*.

Since every interesting trajectory in this system follows the same basic periodic trajectory, this picture represents how the variational integrator behaves for all trajectories except the only fixed point at the origin. $\square$

In the simple harmonic oscillator, all of the trajectories aside from the fixed point have the same behavior of periodicity about the origin. We thus consider a slightly more complicated case of the pendulum.

Example 5.2.4. Recall that the Lagrangian is

$$L(q, \dot{q}) = \frac{1}{2}ml^2\dot{q}^2 + mgl \cos q.$$

The reader can verify that, using the same quadrature and integrator, the discrete system is

$$\begin{aligned} q_{k+1} &= q_k + \frac{hp_{k+1}}{ml^2} \\ p_{k+1} &= p_k - hmg \sin q_k. \end{aligned}$$

Plotting the return maps using several initial points in the different regions we know, a priori, to have different behavior, we obtain Fig. 5.4. Thus, plotting the projection of the phase space of the pendulum in a strip $[-\pi, \pi) \times \mathbb{R}$ via the variational integrator, we have Fig. 5.5, which turns out to be almost² a qualitative copy of the phase space of the original system. $\square$

Lastly, an observant reader may have noticed that in all of the figures demonstrating the periodicity of the variational integrator, the distance between the initial point and each of the return maps look periodic. This appears to not be coincidental. We suspect it to be an artifact of the finite precision of the representation of numbers in computers. That is, finiteness of the number of digits of the frequency vector implies that the Diophantine

² The only trajectories that do not appear to have an appropriate analog are the two that approach the unstable equilibria as $t \rightarrow \infty$, as illustrated in Fig. 5.5.

condition (Eq. (4.4)) is never truly satisfied when we implement the variational integrator, or any symplectic one-step method, in the computer.

Figure 5.4: Distance between the n th return map and the initial point of the trajectory, as a function of n . This uses the variational integrator applied to the pendulum at six different initial points. Top left: $(0, 0.5)$. Top right: $(0, 1)$. Middle left: $(0, 1.5)$. Middle right: $(0, 2)$. Bottom left: $(0, 2.5)$. Bottom right: $(0, 3)$. Notice that, again, the distances are measured on the scale of $1e-5$.

Figure 5.5: The phase space produced by the variational integrator applied to the pendulum.

CHAPTER 6

CLOSING THOUGHTS AND OPEN QUESTIONS

We have but briefly outlined the prerequisites and the sequence leading to the results obtained by West ([Wes04]) and O’Neale ([O’N09]). We have seen that in the transition from continuous Hamiltonian systems to discrete systems via variational integrators, periodicity of trajectories is preserved via a KAM-type theorem. This is only a small facet of several more general questions.

What is the behavior of the remaining types of discrete trajectories produced by variational integrators? In other words, if the original trajectory obtained from the Hamiltonian system is periodic, what are the effects of the variational integrator when the frequency is resonant or almost resonant? O’Neale ([O’N09]) gave a brief sketch of possibilities, which we encourage the reader to explore.

Is it possible to extend the theorems stated by Moan ([Moa04]) and Pronin and Treschev ([PT97]) to multi-step symplectic integrators? Unfortunately, the partial answer appears to be no. Tang proved ([Tan93]) a conjecture of Feng ([Fen86]) that all linear multi-step methods cannot be symplectic. For symplecticity to hold, Tang showed in the same paper that the integrators must be of order two.

The next logical question is then to find the sufficient conditions for the original continuous trajectories such that variational integrators produce discrete periodic trajectories. Armed with such a theorem, we can then proceed to determine whether the original trajectories are periodic or not, given that the discrete trajectory is periodic.

Fixed points and periodic trajectories are but an extremely small subset of range of behavior that can occur in a Hamiltonian system. Thus, the overarching question is, is it possible to extend the theorems we explored such that the discrete trajectory remains

qualitatively similar in behavior to the original trajectory?

An immediate pressing need is the well-definedness of the question. Thus, to proceed, one will need to state the types of comparisons that can be formulated between discrete and continuous trajectory. One way is to simply embed the discrete trajectory in an additional time-like dimension, a la Moan ([Moa04]), and form interpolations between successive points in the discrete trajectory. However, one can also quantify the question by using other quantities that share similar definitions between discrete and continuous trajectories, such as the Lyapunov exponent.

In such scenarios, it appears that KAM theory does not apply, due to the general lack of invariant tori. However, symplectic one-step methods are but a small subset of numerical integrators; thus it is possible to explore such questions by developing numerical integrators that preserve other physical quantities than symplecticity.

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