
This is an electronic reprint of the original article.
This reprint may differ from the original in pagination and typographic detail.

Burby, J. W.; Hirvijoki, E.; Leok, M.

Nearly Periodic Maps and Geometric Integration of Noncanonical Hamiltonian Systems

Published in:
Journal of Nonlinear Science

DOI:
[10.1007/s00332-023-09891-4](https://doi.org/10.1007/s00332-023-09891-4)

Published: 01/04/2023

Document Version
Publisher's PDF, also known as Version of record

Published under the following license:
CC BY

Please cite the original version:
Burby, J. W., Hirvijoki, E., & Leok, M. (2023). Nearly Periodic Maps and Geometric Integration of Noncanonical Hamiltonian Systems. *Journal of Nonlinear Science*, 33(2), Article 38. <https://doi.org/10.1007/s00332-023-09891-4>



Nearly Periodic Maps and Geometric Integration of Noncanonical Hamiltonian Systems

J. W. Burby¹ · E. Hirvijoki² · M. Leok³

Received: 10 January 2022 / Accepted: 21 January 2023
© The Author(s) 2023

Abstract

M. Kruskal showed that each continuous-time nearly periodic dynamical system admits a formal $U(1)$ -symmetry, generated by the so-called roto-rate. When the nearly periodic system is also Hamiltonian, Noether's theorem implies the existence of a corresponding adiabatic invariant. We develop a discrete-time analog of Kruskal's theory. Nearly periodic maps are defined as parameter-dependent diffeomorphisms that limit to rotations along a $U(1)$ -action. When the limiting rotation is non-resonant, these maps admit formal $U(1)$ -symmetries to all orders in perturbation theory. For Hamiltonian nearly periodic maps on exact presymplectic manifolds, we prove that the formal $U(1)$ -symmetry gives rise to a discrete-time adiabatic invariant using a discrete-time extension of Noether's theorem. When the unperturbed $U(1)$ -orbits are contractible, we also find a discrete-time adiabatic invariant for mappings that are merely presymplectic, rather than Hamiltonian. As an application of the theory, we use it to develop a novel technique for geometric integration of non-canonical Hamiltonian systems on exact symplectic manifolds.

Contents

| | | |
|-----|---|-------|
| 1 | Introduction | |
| 1.1 | Notational Conventions | |
| 2 | Overview | |
| 3 | Kruskal's Theory of Nearly Periodic Systems | |
| 4 | Nearly Periodic Maps | |

Communicated by Anthony Bloch.

✉ J. W. Burby
jburby@lanl.gov

¹ Los Alamos National Laboratory, Los Alamos, NM 87545, USA

² Department of Mechanical Engineering, Aalto University, PO Box 14400, 00076 Espoo, Finland

³ Department of Mathematics, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093-0112, USA

| | |
|-----|--|
| 4.1 | Nearly Periodic Maps With Hamiltonian Structure |
| 4.2 | Geometric Integration of Noncanonical Hamiltonian Systems Using Nearly Periodic Maps |
| 5 | Examples |
| 5.1 | Hidden-Variable Newtonian Gravity |
| 5.2 | Reduced Guiding-Center Motion |
| 6 | Discussion |
| | References |

1 Introduction

A continuous-time dynamical system with vector parameter γ is nearly periodic if all of its trajectories are periodic with nowhere-vanishing angular frequency in the limit $\gamma \rightarrow 0$. Examples from physics include charged particle dynamics in a strong magnetic field, the weakly relativistic Dirac equation, and any mechanical system subject to a high-frequency, time-periodic force. In the broader context of multi-scale dynamical systems, nearly periodic systems play a special role because they display perhaps the simplest possible non-dissipative short-timescale dynamics. They therefore provide a useful proving ground for analytical and numerical methods aimed at more complex multi-scale models.

In a seminal paper (Kruskal 1962), Kruskal deduced the basic asymptotic properties of continuous-time nearly periodic systems. In general, each such system admits a formal $U(1)$ -Lie symmetry whose infinitesimal generator R_γ is known as the roto-rate. In the Hamiltonian setting, existence of the roto-rate implies existence of an all-orders adiabatic invariant μ_γ by way of Noether's theorem. General expressions for μ_γ may be found in Burby and Squire (2020). Recently (Burby and Hirvijoki 2021), we extended Kruskal's analysis by proving that the (formal) set of fixed points for the roto-rate is an elliptic almost invariant slow manifold. Moreover, in the Hamiltonian case, we demonstrated that normal stability of the slow manifold is mediated by Kruskal's adiabatic invariant.

The purpose of this article is to introduce discrete-time analogs of continuous-time nearly periodic systems that we call nearly periodic maps. These objects can be motivated as follows. A nearly periodic system characteristically displays limiting short-timescale dynamics that ergodically covers circles in phase space. This ergodicity is ultimately what gives rise to Kruskal's roto-rate and, in the presence of Hamiltonian structure, adiabatic invariance. It is therefore sensible to regard parameter-dependent maps whose limiting iterations ergodically cover circles as discrete-time analogs of nearly periodic systems. Ergodicity requires that the rotation angle associated with each circle be an irrational multiple of 2π . In principle, these rotation angles could vary from circle to circle, but smoothness removes this freedom and imposes a common rotation angle across circles. Nearly periodic maps are defined by limiting iterations that rotate a family of circles foliating phase space by a common rotation angle. Such a map is resonant or non-resonant when the rotation angle is a rational or irrational multiple of 2π , respectively. The preceding remarks suggest that non-resonant nearly periodic maps should share important features with continuous-time nearly periodic systems.

We will show that non-resonant nearly periodic maps always admit formal $U(1)$ -symmetries by modifying Kruskal's construction of a normal form for the roto-rate. Thus, non-resonant nearly periodic maps formally reduce to mappings on the space of $U(1)$ -orbits, corresponding to elimination of a single dimension in phase space. In the Hamiltonian setting, we will establish a discrete-time analog of Noether's theorem that will allow us to construct all-orders adiabatic invariants for non-resonant nearly periodic maps. In contrast to the continuous-time case, there may be topological obstructions to the Noether theorem-based construction. Nevertheless, assuming (a) existence of a fixed point for formal $U(1)$ -symmetry, or (b) existence of a time-dependent Hamiltonian suspension for the nearly periodic map (a time-dependent Hamiltonian flow that interpolates between the identity and the nearly periodic map), these topological obstructions disappear. When an adiabatic invariant does exist, the phase-space dimension is formally reduced by two instead of one. On the slow manifold, corresponding to vanishing of the adiabatic invariant, the reduction in dimensionality may be even more dramatic.

We anticipate that non-resonant nearly periodic maps will have important applications to numerical integration of nearly periodic systems. While development of integrators for such systems is straightforward when the numerical timestep h resolves the short-timescale dynamics, considerably more care is required when "stepping over" the period of limiting oscillations. One approach would be to design an integrator on the unreduced space that is constrained to be a non-resonant nearly periodic map. Although such an integrator would not accurately resolve the phase of short-scale oscillations when taking large timesteps, it would automatically possess an all-orders reduction to the space of $U(1)$ -orbits. By designing the reduced map to discretize the continuous-time reduced dynamics, the slow component of the continuous-time dynamics could be accurately resolved without directly simulating the reduced dynamical variables. This opens the door to a type of asymptotic-preserving integrator capable of seamlessly transitioning between large- and small-timestep regimes, generalizing those proposed in Ricketson and Chacón (2020), Xiao and Qin (2021) for magnetized charged particle dynamics. Moreover, in the Hamiltonian case, the integrator would automatically enjoy an all-orders adiabatic invariant close to the continuous-time invariant. Such a capability would complement previous results on short-timestep adiabatic invariants for variational integrators (Hairer and Lubich 2020). We provide a proof-of-principle demonstration of these ideas in Sect. 5.1

Aside from serving as integrators for nearly periodic systems, nearly periodic maps may also be used as tools for structure-preserving simulation of general Hamiltonian systems on exact symplectic manifolds. (See Abraham and Marsden 2008; Marsden and Ratiu 1999 for the foundations of Hamiltonian mechanics on symplectic manifolds.) The basic idea is to first embed the original Hamiltonian system as an approximate invariant manifold inside of a larger nearly periodic Hamiltonian system, as discussed in Burby and Hirvijoki (2021). Then, it is possible to construct a symplectic nearly periodic map that integrates the larger system while preserving the approximate invariant manifold. Discrete-time adiabatic invariance ensures that the approximate invariant manifold enjoys long-term normal stability, which is tantamount to the integrator providing a persistent approximation of the original system's dynamics. We describe and analyze this construction in Sect. 4.2. In Sect. 5.2, we apply

the general theory to the non-canonical Hamiltonian dynamics of a charged particle's guiding center (Northrop 1963; Littlejohn 1981, 1983) in a magnetic field of the form $\mathbf{B} = B(x, y) \mathbf{e}_z$ (Littlejohn 1979).

The remainder of this article is organized as follows. After providing a brief non-technical overview, we review Kruskal's theory of nearly periodic systems using modern terminology in Sect. 3. Then, we develop the general theory of nearly periodic maps in Sect. 4, including their special properties in the symplectic case, and their ability to serve as geometric integrators for Hamiltonian systems on exact symplectic manifolds. Wherever possible, proofs of general properties of nearly periodic maps parallel Kruskal's arguments from the continuous-time setting. Section 5 contains a pair of interesting applications of nearly periodic map technology. Finally, Sect. 6 provides additional review and context for this work.

1.1 Notational Conventions

In this article, smooth shall always mean C^∞ , and Γ will always denote a vector space. We reserve the symbol M for a smooth manifold equipped with a smooth auxiliary Riemannian metric g . We say $f_\gamma : M_1 \rightarrow M_2$, $\gamma \in \Gamma$, is a smooth γ -dependent mapping between manifolds M_1, M_2 when the mapping $M_1 \times \mathbb{R} \rightarrow M_2 : (m, \gamma) \mapsto f_\gamma(m)$ is smooth. Similarly, T_γ is a smooth γ -dependent tensor field on M when (a) $T_\gamma(m)$ is an element of the tensor algebra $\mathcal{T}_m(M)$ at m for each $m \in M$ and $\gamma \in \Gamma$, and (b) T_γ is a smooth γ -dependent mapping between the manifolds M and $\mathcal{T}(M) = \bigcup_{m \in M} \mathcal{T}_m(M)$.

The symbol X_γ will always denote a smooth γ -dependent vector field on M . If T_γ is a smooth γ -dependent section of either $TM \otimes TM$ or $T^*M \otimes T^*M$, then \widehat{T}_γ is the corresponding smooth γ -dependent bundle map $T^*M \rightarrow TM : \alpha \mapsto \iota_\alpha T_\gamma$, or $TM \rightarrow T^*M : X \mapsto \iota_X T_\gamma$, respectively. Note that if Ω is a symplectic form on M with associated Poisson bivector \mathcal{J} then $\widehat{\Omega}^{-1} = -\widehat{\mathcal{J}}$. Finally, we introduce the following definition to address presymplectic forms that depend on a parameter.

Definition 1 Let $\Gamma \ni \gamma$ be a finite-dimensional vector space. A γ -**dependent presymplectic manifold** is a manifold M equipped with a smooth γ -dependent 2-form Ω_γ such that $\mathbf{d}\Omega_\gamma = 0$ for each $\gamma \in \Gamma$. We say (M, Ω_γ) is **exact** when there is a smooth γ -dependent 1-form ϑ_γ such that $\Omega_\gamma = -\mathbf{d}\vartheta_\gamma$.

2 Overview

This article contains a pair of interrelated contributions, an analog of Kruskal's nearly periodic system theory in discrete time, and an application of the new theory to structure-preserving integration of non-canonical Hamiltonian systems. Each contribution requires understanding a fair amount of technical background material to fully digest. This section therefore aims to present a (mostly) non-technical synopsis of our work. Readers interested in proceeding directly to the technical content should start with Sect. 3.

Kruskal's theory Kruskal (1962) represented an outgrowth of vigorous investigations into charged particle motion in strong magnetic fields as part of Project Matterhorn, the first serious attempt by the US government to develop nuclear fusion for peaceful energy production. Such charged particles execute rapid rotation around magnetic field lines superposed on a much slower drift motion. Moreover, the magnetic flux that threads their tight helical trajectories remains approximately constant in time over large time intervals, almost as if each particle behaved as a superconducting ring of current. Kruskal recognized that this problem comprised just one example of a rich class of multi-scale dynamical systems for which much could be said using analytical methods. These systems, now called nearly periodic, exhibit two time scales, a short one on which every trajectory is periodic, and a much longer one associated with slow drifting motion. Kruskal also recognized that the magnetic flux invariant from charged particle theory generalizes to nearly periodic systems *provided* the nearly periodic system admits Hamiltonian structure.

Nearly periodic systems bear similarities with the nearly integrable systems addressed by Kolmogorov–Arnol'd–Moser (KAM) theory. They depend on a small parameter ϵ that measures a degree of timescale separation. When $\epsilon \rightarrow 0$, all trajectories become very simple—even explicitly integrable in the right coordinate system. In fact, nearly periodic systems may be viewed as special examples of nearly integrable systems. However, where nearly integrable systems generically exhibit resonances nearly periodic systems never do. The limiting dynamics for a nearly integrable Hamiltonian system comprise quasiperiodic motion on invariant Lagrangian tori in phase space characterized by several fast phases. On many of these tori, the fast frequencies exhibit integer relationships that notoriously cause perturbation series to break down. But for a nearly periodic system the tori are one-dimensional, making resonance impossible. Kruskal exploited this lack of obstruction to perturbative methods to prove a remarkable result: every nearly periodic system admits a unique hidden continuous symmetry at the level of perturbation theory. While Kruskal did not prove that the series defining his symmetry converge or represent a genuine symmetry in any sense, formal existence and uniqueness proved sufficient to explain the magnetic flux invariant for charged particles, and more generally adiabatic invariants in any nearly periodic system.

A simple consequence of the existence of a formal hidden symmetry and corresponding adiabatic invariant for a nearly periodic Hamiltonian system is existence of a non-trivial class of phase space diffeomorphisms with hidden symmetries and adiabatic invariants. At a minimum, this class contains the time- t flow maps for nearly periodic Hamiltonian systems, for any value of t . The work presented in this article emerged from a desire to better understand this interesting class of maps. Following Kruskal's lead, our goal was to first define these maps axiomatically and then transcribe Kruskal's arguments to the extent possible in order to prove they have the right properties. Section 4 represents the successful culmination of this effort.

Our theory of discrete-time nearly periodic systems, or nearly periodic maps for brevity, largely parallels Kruskal's original theory in continuous time. But there is one key technical challenge that appears in discrete time and not in continuous time, which can be described as follows. Ultimately, perturbation theory for dynamical systems involves integration along unperturbed trajectories. For a continuous-time

nearly periodic system, such integrations manifest themselves in the form of partial differential equations of the general type

$$\omega(x) \partial_{\theta} f(x, \theta) = S(x, \theta), \quad x \in \mathbb{R}^n, \quad \theta \in \mathbb{R} \bmod 2\pi$$

where the source function $S(x, \theta)$ and the (assumed nowhere vanishing) angular frequency $\omega(x)$ are known and $f(x, \theta)$ is the dependent variable. Provided the θ -average of S vanishes, this equation yields to solution by the method of Fourier series. No resonances appear. For nearly periodic maps, integrating along unperturbed orbits instead leads to functional equations of the form

$$f(x, \theta + \theta_0) - f(x, \theta) = S(x, \theta), \quad x \in \mathbb{R}^n, \quad \theta \in \mathbb{R} \bmod 2\pi$$

where θ_0 is a constant parameter characterizing the map's limiting rotation angle. Fourier analysis in θ reveals that solving for the n^{th} Fourier coefficient f_n requires division by $1 - \exp(i n \theta)$. This step becomes problematic whenever $\theta = 2\pi q$, where q is a rational number. Of course, this issue may be avoided formally by choosing the limiting rotation angle to be an irrational fraction of 2π . But the possibility of resonance remains in the theory, leading to a dichotomy between resonant and non-resonant nearly periodic maps. Most of Kruskal's arguments transcribe nicely to discrete time in the non-resonant case only.

In light of our recent results from Burby and Hirvijoki (2021), existence of nearly periodic maps presented interested possibilities for important applications of our theory. For example, we showed that every Hamiltonian system on an exact symplectic manifold embeds as a slow manifold for a larger nearly periodic system with a simple Hamiltonian structure. Due to the close relationship between flow maps for nearly periodic systems and nearly periodic maps, this suggests that nearly periodic maps might be useful for simulating a very broad class of Hamiltonian systems without the need for first identifying canonical variables. Section 4.2 shows that this hunch is actually correct. Given a possibly non-canonical Hamiltonian system, we first embed the dynamics as a slow manifold in a nearly periodic Hamiltonian system using the construction from Burby and Hirvijoki (2021). Then, we construct a nearly periodic map that preserves the Hamiltonian structure of the larger system and approximately integrates the nearly periodic flow. By restricting such an integrator to initial conditions that lie on the zero level set of the map's adiabatic invariant (guaranteed by the general theory of nearly periodic maps), we obtain an effective structure-preserving integrator for the original Hamiltonian dynamics. No canonical variables required.

3 Kruskal's Theory of Nearly Periodic Systems

In 1962, Kruskal presented an asymptotic theory (Kruskal 1962) of averaging for dynamical systems whose trajectories are all periodic to leading order. Nowadays, Kruskal's method is termed one-phase averaging (Lochak 1993), which suggests a contrast with the multi-phase averaging methods underlying, e.g., KAM theory. Since this theory provides a model for the results in this article, we review its main ingredients

here. In this section only, and merely for simplicity's sake, we make the restriction $\Gamma = \mathbb{R}$.

Definition 2 A **nearly periodic system** on a manifold M is a smooth γ -dependent vector field X_γ on M such that $X_0 = \omega_0 R_0$, where

- $\omega_0 : M \rightarrow \mathbb{R}$ is strictly positive
- R_0 is the infinitesimal generator for a circle action $\Phi_\theta : M \rightarrow M$, $\theta \in U(1)$.
- $\mathcal{L}_{R_0} \omega_0 = 0$.

The vector field R_0 is called the **limiting roto-rate**, and ω_0 is the **limiting angular frequency**.

Remark 1 In addition to requiring that ω_0 is sign-definite, Kruskal assumed that R_0 is nowhere vanishing. However, this assumption is not essential for one-phase averaging to work. It is enough to require that ω_0 vanishes nowhere. This is an important restriction to lift since many interesting circle actions have fixed points.

Kruskal's theory applies to both Hamiltonian and non-Hamiltonian systems. In the Hamiltonian setting, it leads to stronger conclusions. A general class of Hamiltonian systems for which the theory works nicely may be defined as follows.

Definition 3 Let (M, Ω_γ) be a manifold equipped with a smooth γ -dependent presymplectic form Ω_γ . Assume there is a smooth γ -dependent 1-form ϑ_γ such that $\Omega_\gamma = -\mathbf{d}\vartheta_\gamma$. A **nearly periodic Hamiltonian system** on (M, Ω_γ) is a nearly periodic system X_γ on M such that $\iota_{X_\gamma} \Omega_\gamma = \mathbf{d}H_\gamma$, for some smooth γ -dependent function $H_\gamma : M \rightarrow \mathbb{R}$.

Kruskal showed that all nearly periodic systems admit an approximate $U(1)$ -symmetry that is determined to leading order by the unperturbed periodic dynamics. He named the generator of this approximate symmetry the *roto-rate*. In the Hamiltonian setting, he showed that both the dynamics and the Hamiltonian structure are $U(1)$ -invariant to all orders in γ .

Definition 4 A **roto-rate** for a nearly periodic system X_γ on a manifold M is a formal power series $R_\gamma = R_0 + \gamma R_1 + \gamma^2 R_2 + \dots$ with vector field coefficients such that

- R_0 is equal to the limiting roto-rate
- $\exp(2\pi \mathcal{L}_{R_\gamma}) = 1$
- $[X_\gamma, R_\gamma] = 0$,

where the second and third conditions are understood in the sense of formal power series.

Proposition 1 (Kruskal (1962)) *Every nearly periodic system admits a unique roto-rate R_γ . The roto-rate for a nearly periodic Hamiltonian system on an exact presymplectic manifold (M, Ω_γ) satisfies $\mathcal{L}_{R_\gamma} \Omega_\gamma = 0$ in the sense of formal power series.*

Corollary 1 *The roto-rate R_γ for a nearly periodic Hamiltonian system X_γ on an exact presymplectic manifold (M, Ω_γ) with Hamiltonian H_γ satisfies $\mathcal{L}_{R_\gamma} H_\gamma = 0$.*

Proof Since $[R_\gamma, X_\gamma] = \mathcal{L}_{R_\gamma} X_\gamma = 0$ and $\mathcal{L}_{R_\gamma} \Omega_\gamma = 0$, we may apply the Lie derivative \mathcal{L}_{R_γ} to Hamilton's equation $\iota_{X_\gamma} \Omega_\gamma = \mathbf{d}H_\gamma$ to obtain

$$\mathcal{L}_{R_\gamma}(\mathbf{d}H_\gamma) = \mathcal{L}_{R_\gamma}(\iota_{X_\gamma} \Omega_\gamma) = \iota_{\mathcal{L}_{R_\gamma} X_\gamma} \Omega_\gamma + \iota_{X_\gamma}(\mathcal{L}_{R_\gamma} \Omega_\gamma) = 0.$$

Thus, $\mathcal{L}_{R_\gamma} H_\gamma$ is a constant function. By averaging over the $U(1)$ -action we conclude that the constant must be zero. \square

To prove Proposition 1, Kruskal used a pair of technical results, each of which is interesting in its own right. The first establishes the existence of a non-unique normalizing transformation that asymptotically deforms the $U(1)$ -action generated by R_γ into the simpler $U(1)$ -action generated by R_0 . The second is a subtle bootstrapping argument that upgrades leading-order $U(1)$ -invariance to all-orders $U(1)$ -invariance for integral invariants. We state these results here for future reference.

Definition 5 Let $G_\gamma = \gamma G_1 + \gamma^2 G_2 + \dots$ be an $O(\gamma)$ (no constant term) formal power series whose coefficients are vector fields on a manifold M . The **Lie transform** with **generator** G_γ is the formal power series $\exp(\mathcal{L}_{G_\gamma})$ whose coefficients are differential operators on the tensor algebra over M .

Definition 6 A **normalizing transformation** for a nearly periodic system X_γ with roto-rate R_γ is a Lie transform $\exp(\mathcal{L}_{G_\gamma})$ with generator G_γ such that $R_\gamma = \exp(\mathcal{L}_{G_\gamma}) R_0$.

Proposition 2 (Kruskal) *Each nearly periodic system admits a normalizing transformation.*

Proposition 3 *Let α_γ be a smooth γ -dependent differential form on a manifold M . Suppose α_γ is an absolute integral invariant for a C^∞ nearly periodic system X_γ on M . If $\mathcal{L}_{R_0} \alpha_0 = 0$ then $\mathcal{L}_{R_\gamma} \alpha_\gamma = 0$, where R_γ is the roto-rate for X_γ .*

Proof Integral invariance means $\mathcal{L}_{X_\gamma} \alpha_\gamma = 0$ for each $\gamma \in \Gamma$. By Applying \mathcal{L}_{R_γ} to this relationship, and using $[R_\gamma, X_\gamma] = 0$, we obtain $\mathcal{L}_{X_\gamma} \mathcal{L}_{R_\gamma} \alpha_\gamma = 0$. Now let G_γ be the generator of a normalizing transformation for X_γ , and set $\bar{X}_\gamma = \exp(-\mathcal{L}_{G_\gamma}) X_\gamma$, $\bar{\alpha}_\gamma = \exp(-\mathcal{L}_{G_\gamma}) \alpha_\gamma$. We have $\mathcal{L}_{\bar{X}_\gamma} \mathcal{L}_{R_0} \bar{\alpha}_\gamma = 0$. Since $\mathcal{L}_{R_0} \bar{\alpha}_\gamma = O(\gamma)$, the first-order consequence of the previous formula is $\mathcal{L}_{\omega_0 R_0} \mathcal{L}_{R_0} \bar{\alpha}_1 = 0$, which can only be satisfied if $\mathcal{L}_{R_0} \bar{\alpha}_1$ is R_0 -invariant. But since the $U(1)$ -average of $\mathcal{L}_{R_0} \bar{\alpha}_1$ vanishes, we conclude $\mathcal{L}_{R_0} \bar{\alpha}_1 = 0$. Repeating this argument gives $\mathcal{L}_{R_0} \bar{\alpha}_k = 0$ for $k > 1$ as well. In other words $\mathcal{L}_{R_0} \bar{\alpha}_\gamma = 0$ to all orders in γ , which is equivalent to the theorem's claim. \square

According to Noether's celebrated theorem, a Hamiltonian system that admits a continuous family of symmetries also admits a corresponding conserved quantity. Therefore, one might expect that a Hamiltonian system with approximate symmetry must also have an approximate conservation law. Kruskal showed that this is indeed the case for nearly periodic Hamiltonian systems, as the following generalization of his argument shows.

Proposition 4 Let X_γ be a nearly periodic Hamiltonian system on the exact presymplectic manifold (M, Ω_γ) . Let R_γ be the associated roto-rate. There is a formal power series $\theta_\gamma = \theta_0 + \gamma \theta_1 + \dots$ with coefficients in $\Omega^1(M)$ such that $\Omega_\gamma = -\mathbf{d}\theta_\gamma$ and $\mathcal{L}_{R_\gamma}\theta_\gamma = 0$. Moreover, the formal power series $\mu_\gamma = \iota_{R_\gamma}\theta_\gamma$ is a constant of motion for X_γ to all orders in perturbation theory. In other words,

$$\mathcal{L}_{X_\gamma}\mu_\gamma = 0,$$

in the sense of formal power series.

Proof To construct the $U(1)$ -invariant primitive θ_γ , we select an arbitrary primitive ϑ_γ for Ω_γ and set

$$\theta_\gamma = \frac{1}{2\pi} \int_0^{2\pi} \exp(\theta \mathcal{L}_{R_\gamma}) \vartheta_\gamma d\theta.$$

This formal power series satisfies $\mathcal{L}_{R_\gamma}\theta_\gamma = 0$ because

$$\mathcal{L}_{R_\gamma}\theta_\gamma = \frac{1}{2\pi} \int_0^{2\pi} \frac{d}{d\theta} \exp(\theta \mathcal{L}_{R_\gamma}) \vartheta_\gamma d\theta = 0.$$

Moreover, since $\mathcal{L}_{R_\gamma}\Omega_\gamma = 0$ by Kruskal's Proposition 1, we have

$$-\mathbf{d}\theta_\gamma = \frac{1}{2\pi} \int_0^{2\pi} \exp(\theta \mathcal{L}_{R_\gamma}) \Omega_\gamma d\theta = \frac{1}{2\pi} \int_0^{2\pi} \Omega_\gamma d\theta = \Omega_\gamma,$$

whence θ_γ is a primitive for Ω_γ .

To establish all-orders time independence of $\mu_\gamma = \iota_{R_\gamma}\theta_\gamma$, we apply Cartan's formula and Corollary 1 according to

$$\mathcal{L}_{X_\gamma}\mu_\gamma = \iota_{X_\gamma}\mathbf{d}\iota_{R_\gamma}\theta_\gamma = -\iota_{R_\gamma}\iota_{X_\gamma}\Omega_\gamma = -\mathcal{L}_{R_\gamma}H_\gamma = 0.$$

□

Definition 7 The formal constant of motion μ_γ provided by Proposition 4 is the **adiabatic invariant** associated with a nearly periodic Hamiltonian system.

4 Nearly Periodic Maps

Nearly periodic maps are natural discrete-time analogs of nearly periodic systems. The following provides a precise definition.

Definition 8 (nearly periodic map) Let Γ be a vector space. A **nearly periodic map** on a manifold M with parameter space Γ is a smooth mapping $F : M \times \Gamma \rightarrow M$ such that $F_\gamma : M \rightarrow M : m \mapsto F(m, \gamma)$ has the following properties:

- F_γ is a diffeomorphism for each $\gamma \in \Gamma$.
- There exists a $U(1)$ -action $\Phi_\theta : M \rightarrow M$ and a constant $\theta_0 \in U(1)$ such that $F_0 = \Phi_{\theta_0}$.

We say F is **resonant** if θ_0 is a rational multiple of 2π , otherwise F is **non-resonant**. The infinitesimal generator of Φ_θ , R_0 , is the **limiting roto-rate**.

Let X be a vector field on a manifold M with time- t flow map \mathcal{F}_t . A $U(1)$ -action Φ_θ is a symmetry for X if $\mathcal{F}_t \circ \Phi_\theta = \Phi_\theta \circ \mathcal{F}_t$, for each $t \in \mathbb{R}$ and $\theta \in U(1)$. Differentiating this condition with respect to θ at the identity implies $\mathcal{F}_t^* R = R$, where R denotes the infinitesimal generator for the $U(1)$ -action. Conversely, if R is any vector field with 2π -periodic orbits and $\mathcal{F}_t^* R = R$ for each $t \in \mathbb{R}$ then the R -flow defines a $U(1)$ -action that is a symmetry for X . Since we would like to think of nearly periodic maps as playing the part of a nearly periodic system's flow map, the latter characterization of symmetry allows us to naturally extend Kruskal's notion of roto-rate to our discrete-time setting.

Definition 9 A **roto-rate** for a nearly periodic map F is a formal power series $R_\gamma = R_0 + R_1[\gamma] + R_2[\gamma, \gamma] + \dots$ whose coefficients are homogeneous polynomial maps from Γ into vector fields on M such that

- R_0 is the limiting roto-rate.
- $F_\gamma^* R_\gamma = R_\gamma$ in the sense of formal power series.
- $\exp(2\pi \mathcal{L}_{R_\gamma}) = 1$ in the sense of formal power series.

Definition 10 Let $G_\gamma = G_1[\gamma] + G_2[\gamma, \gamma] + \dots$ be an $O(\gamma)$ (no constant term) formal power series whose coefficients are homogeneous polynomial maps from Γ into vector fields on M . The **Lie transform** with **generator** G_γ is the formal power series $\exp(\mathcal{L}_{G_\gamma})$ whose coefficients are homogeneous polynomial maps from Γ into differential operators on the tensor algebra over M .

Remark 2 Since the parameter γ in the previous two definitions is vector valued, the formal power series R_γ and G_γ may be usefully interpreted as multivariate formal power series.

Definition 11 A **normalizing transformation** for a nearly periodic map F with roto-rate R_γ is a Lie transform $\exp(\mathcal{L}_{G_\gamma})$ with generator G_γ such that $R_\gamma = \exp(\mathcal{L}_{G_\gamma}) R_0$.

Our first and most fundamental result concerning nearly periodic maps establishes the existence and uniqueness of the roto-rate in the non-resonant case. Like the corresponding result due to Kruskal in continuous time, this result holds to all orders in perturbation theory.

Theorem 1 (Existence and uniqueness of the roto-rate) *Each non-resonant nearly periodic map admits a unique roto-rate.*

Proof First we will show that there exists a Lie transform with generator G_γ such that $R_\gamma \equiv \exp(\mathcal{L}_{G_\gamma}) R_0$ is a roto-rate.

To that end, we introduce a convenient way of representing γ -dependent pullback operators at the level of formal power series. Let ψ_γ be a smooth γ -dependent diffeomorphism on M . By the Lie derivative formula, there is a unique γ -dependent Γ^* -valued vector field W_γ such that

$$\left. \frac{d}{ds} \right|_{s=0} \psi_{\gamma+s\delta\gamma}^* = \psi_\gamma^* \mathcal{L}_{\langle W_\gamma, \delta\gamma \rangle}, \quad (1)$$

for each $\gamma, \delta\gamma \in \Gamma$. Here $\langle \cdot, \cdot \rangle$ denotes the natural pairing between Γ and its dual space Γ^* . The object W_γ both determines and is determined by the pullback operator ψ_γ^* at the level of formal power series. This follows from recursive application of the identity

$$\psi_{s\gamma}^* = \psi_0^* + \int_0^s \psi_{s_1\gamma}^* \mathcal{L}_{\langle W_{s_1\gamma}, \gamma \rangle} ds_1, \quad (2)$$

which may be understood as a consequence of (1) and the fundamental theorem of calculus. This can be viewed as Picard iteration of (1) or fixed point iteration of (2). The first step in the recursion is to substitute (2) with $s = s_1$ into (2) with $s = 1$, resulting in

$$\begin{aligned} \psi_\gamma^* &= \psi_0 + \int_0^1 \left(\psi_0^* + \int_0^{s_1} \psi_{s_2\gamma}^* \mathcal{L}_{\langle W_{s_2\gamma}, \gamma \rangle} ds_2 \right) \mathcal{L}_{\langle W_{s_1\gamma}, \gamma \rangle} ds_1 \\ &= \psi_0 + \int_0^1 \psi_0^* \mathcal{L}_{\langle W_{s_1\gamma}, \gamma \rangle} ds_1 + \int_0^1 \int_0^{s_1} \psi_{s_2\gamma}^* \mathcal{L}_{\langle W_{s_2\gamma}, \gamma \rangle} \mathcal{L}_{\langle W_{s_1\gamma}, \gamma \rangle} ds_2 ds_1. \end{aligned}$$

The second step involves substituting (2) with $s = s_2$ into the preceding expression, thereby producing a triple integral. Continuing in this manner, it is straightforward to derive the following time-ordered exponential formulas for both the pullback ψ_γ^* and pushforward operator $\psi_{\gamma*}$,

$$\psi_\gamma^* = \psi_0^* \left[1 + \int_0^1 \mathcal{L}_{\langle W_{s_1\gamma}, \gamma \rangle} ds_1 + \int_0^1 \int_0^{s_1} \mathcal{L}_{\langle W_{s_2\gamma}, \gamma \rangle} \mathcal{L}_{\langle W_{s_1\gamma}, \gamma \rangle} ds_2 ds_1 + \dots \right] \quad (3)$$

$$\psi_{\gamma*} = \left[1 - \int_0^1 \mathcal{L}_{\langle W_{s_1\gamma}, \gamma \rangle} ds_1 + \int_0^1 \int_0^{s_1} \mathcal{L}_{\langle W_{s_1\gamma}, \gamma \rangle} \mathcal{L}_{\langle W_{s_2\gamma}, \gamma \rangle} ds_2 ds_1 + \dots \right] \psi_{0*}. \quad (4)$$

Upon introducing the formal power series expansion $W_\gamma = W_0 + W_1[\gamma] + W_2[\gamma, \gamma] + \dots$, the integrals in these formulas can be carried out, leading to the somewhat more explicit formulas

$$\psi_\gamma^* = \psi_0^* \left[1 + \mathcal{L}_{\langle W_0, \gamma \rangle} + \frac{1}{2} \mathcal{L}_{\langle W_1[\gamma], \gamma \rangle} + \frac{1}{2} \mathcal{L}_{\langle W_0, \gamma \rangle}^2 + O(\gamma^3) \right] \quad (5)$$

$$\psi_{\gamma*} = \left[1 - \mathcal{L}_{\langle W_0, \gamma \rangle} - \frac{1}{2} \mathcal{L}_{\langle W_1[\gamma], \gamma \rangle} + \frac{1}{2} \mathcal{L}_{\langle W_0, \gamma \rangle}^2 + O(\gamma^3) \right] \psi_{0*}. \quad (6)$$

The preceding discussion applies in particular to $\psi_\gamma^* = F_\gamma^*$. In this case, we will use the symbol V_γ for W_γ . The discussion also applies to the formal pullback operator $\psi_\gamma^* = \phi_\gamma^*$, where

$$\phi_\gamma^* = \exp(\mathcal{L}_{G_\gamma}),$$

as well as its inverse $\phi_{\gamma*} = (\phi_\gamma^*)^{-1}$. In this case we will use ξ_γ in place of W_γ . Thus, we have the defining identities

$$\left. \frac{d}{ds} \right|_{s=0} F_{\gamma+s\delta\gamma}^* = F_\gamma^* \mathcal{L}_{\langle V_\gamma, \delta\gamma \rangle} \quad (7)$$

$$\left. \frac{d}{ds} \right|_{s=0} \phi_{\gamma+s\delta\gamma}^* = \phi_\gamma^* \mathcal{L}_{\langle \xi_\gamma, \delta\gamma \rangle}. \quad (8)$$

We will now establish existence of the Lie transform with generator G_γ by constructing an appropriate ξ_γ . The Lie transform itself can then be constructed using the formulas (3) and (4). Define $R_\gamma = \exp(\mathcal{L}_{G_\gamma})R_0 = \phi_\gamma^*R_0$, where G_γ , or equivalently ξ_γ , is yet to be determined. This R_γ satisfies $\exp(2\pi\mathcal{L}_{R_\gamma}) = 1$ and $R_{\gamma=0} = R_0$ automatically. We will determine the formal power series $\xi_\gamma = \xi_0 + \xi_1[\gamma] + \xi_2[\gamma, \gamma] + \dots$ by requiring $F_\gamma^*R_\gamma = R_\gamma$. If this can be done, then R_γ will be a roto-rate.

The equation we would like to solve is equivalent to

$$(\phi_\gamma^{-1})^* F_\gamma^* \phi_\gamma^* R_0 = R_0, \quad (9)$$

where $(\phi_\gamma^{-1})^* = (\phi_\gamma^*)^{-1}$. Formally, this is just the statement that the “diffeomorphism” $\overline{F}_\gamma = \phi_\gamma \circ F_\gamma \circ \phi_\gamma^{-1}$ preserves the limiting roto-rate R_0 . Instead of solving (9) directly, we will demand that its γ -derivative vanishes. This derivative condition is

$$0 = \left. \frac{d}{ds} \right|_{s=0} \overline{F}_{\gamma+s\delta\gamma}^* R_0 = \overline{F}_\gamma^* \mathcal{L}_{\langle \overline{V}_\gamma, \delta\gamma \rangle} R_0, \quad (10)$$

where \overline{V}_γ is readily shown to be given by

$$\overline{V}_\gamma = \xi_\gamma - \overline{F}_\gamma^* \xi_\gamma + \phi_\gamma^* V_\gamma.$$

Note that requiring the γ -derivative of (9) to vanish implies (9) itself since the latter is clearly satisfied when $\gamma = 0$. Also note that since \overline{F}_γ^* is formally invertible, the derivative condition is equivalent to

$$\mathcal{L}_{R_0} \overline{V}_\gamma = 0. \quad (11)$$

To solve (11), we will expand the equation in powers of γ and then argue inductively that each equation in the resulting sequence can be solved. At $O(\gamma^0)$ we have

$$\mathcal{L}_{R_0}(\xi_0 - \Phi_{\theta_0} * \xi_0 + V_0) = 0.$$

Denoting the limiting $U(1)$ -average operation as $\langle T \rangle = (2\pi)^{-1} \int_0^{2\pi} \Phi_{\theta}^* T d\theta$, where T is any tensor field on M , and $T^{\text{osc}} = T - \langle T \rangle$, this equation is equivalent to

$$A_{\theta_0} \xi_0^{\text{osc}} = -V_0^{\text{osc}},$$

where we have introduced the **homological operator**

$$A_{\theta_0} = 1 - \Phi_{\theta_0} *.$$

Since F_{γ} is assumed to be non-resonant, the homological operator, regarded as a linear automorphism of the oscillating subspace of vector fields, is invertible. We may therefore solve the $O(\gamma^0)$ equation by setting

$$\xi_0 = -A_{\theta_0}^{-1} V_0^{\text{osc}}.$$

At $O(\gamma^n)$, (11) leads to

$$A_{\theta_0} \xi_n[\gamma, \dots, \gamma]^{\text{osc}} = S_n[\gamma, \dots, \gamma]^{\text{osc}},$$

where $S_n[\gamma, \dots, \gamma]$ involves coefficients of $V_{\gamma} = V_0 + V_1[\gamma] + V_2[\gamma, \gamma]$ and $\xi_{\gamma} = \xi_0 + \xi_1[\gamma] + \xi_2[\gamma, \gamma] + \dots$ with polynomial degree (for ξ) at most $n-1$. Assuming the ξ_k with $k < n$ have already been determined by solving the $O(\gamma^k)$ components of (11), we may therefore solve the $O(\gamma^n)$ equation by setting

$$\xi_n[\gamma, \dots, \gamma] = A_{\theta_0}^{-1} S_n[\gamma, \dots, \gamma]^{\text{osc}}.$$

Since we have already established that the $O(\gamma^0)$ equation has a solution, we now conclude by induction that (11) may be solved for ξ_{γ} to all orders in γ . It follows that a roto-rate exists.

Next we prove uniqueness of the R_{γ} just constructed. Suppose R'_{γ} is a possibly distinct roto-rate, and consider the commutator $C_{\gamma} = [R_{\gamma}, R'_{\gamma}]$. Immediate properties of C_{γ} include $C_0 = 0$ and $F_{\gamma}^* C_{\gamma} = C_{\gamma}$. By construction of R_{γ} , we have $R_{\gamma} = \exp(\mathcal{L}_{G_{\gamma}}) R_0$, which implies $\bar{C}_{\gamma} = \exp(-\mathcal{L}_{G_{\gamma}}) C_{\gamma} = [R_0, \bar{R}'_{\gamma}]$, where $\bar{R}'_{\gamma} = \exp(-\mathcal{L}_{G_{\gamma}}) R'_{\gamma}$. Thus, the mean $\langle \bar{C}_{\gamma} \rangle = 0$ vanishes to all orders in γ . Since $F_{\gamma}^* C_{\gamma} = C_{\gamma}$, we also have $\bar{F}_{\gamma}^* \bar{C}_{\gamma} = \bar{C}_{\gamma}$, where $\bar{F}_{\gamma}^* \equiv \exp(-\mathcal{L}_{G_{\gamma}}) F_{\gamma}^* \exp(\mathcal{L}_{G_{\gamma}})$. The first-order consequence of the last condition is $\Phi_{\theta_0}^* \bar{C}_1[\gamma] = \bar{C}_1[\gamma]$, which implies $\mathcal{L}_{R_0} \bar{C}_1[\gamma] = 0$ by non-resonance. But since the mean of $\bar{C}_1[\gamma]$ vanishes, we must have $\bar{C}_1[\gamma] = 0$ for all $\gamma \in \Gamma$. The same argument applied repeatedly

implies $\overline{C}_n = 0$ for all $n \geq 1$. In other words, R_γ and R'_γ commute. To finish the argument for uniqueness, we now use commutativity of R_γ and R'_γ to find $1 = \exp(2\pi \mathcal{L}_{R_\gamma}) = \exp(2\pi \mathcal{L}_{R'_\gamma} + 2\pi \mathcal{L}_{R_\gamma - R'_\gamma}) = \exp(2\pi \mathcal{L}_{R_\gamma - R'_\gamma})$, which can only be satisfied if $R_\gamma - R'_\gamma = 0$, since $R_0 - R'_0 = 0$.

□

Theorem 2 (Existence of normalizing transformations) *Each non-resonant nearly periodic map admits a normalizing transformation.*

Proof This follows immediately from the proof of Theorem 1.

□

4.1 Nearly Periodic Maps With Hamiltonian Structure

As in the continuous-time theory, existence of the roto-rate leads to additional insights for nearly periodic maps that are Hamiltonian in an appropriate sense. In this subsection, we will establish the basic properties of nearly periodic maps with Hamiltonian structure. We start by defining what we mean by Hamiltonian structure.

Definition 12 (Presymplectic nearly periodic map) A **Presymplectic nearly periodic map** on a γ -dependent presymplectic manifold (M, Ω_γ) is a nearly periodic map F such that $F_\gamma^* \Omega_\gamma = \Omega_\gamma$ for each $\gamma \in \Gamma$.

Definition 13 (Hamiltonian nearly periodic map) A **Hamiltonian nearly periodic map** on a γ -dependent presymplectic manifold (M, Ω_γ) is a nearly periodic map F such that there is a smooth (t, γ) -dependent vector field $Y_{t,\gamma}$ with the following properties:

- $t \in \mathbb{R}$.
- $\iota_{Y_{t,\gamma}} \Omega_\gamma = dH_{t,\gamma}$, for some smooth (t, γ) -dependent function $H_{t,\gamma}$.
- For each $\gamma \in \Gamma$, F_γ is the $t = 1$ flow of $Y_{t,\gamma}$.

Lemma 1 *Each Hamiltonian nearly periodic map is a presymplectic nearly periodic map.*

Theorem 3 (Roto-rate is presymplectic) *If F is a non-resonant presymplectic nearly periodic map on a γ -dependent presymplectic manifold (M, Ω_γ) with roto-rate R_γ then $\mathcal{L}_{R_\gamma} \Omega_\gamma = 0$.*

Proof First note that presymplecticity of F with $\gamma = 0$ implies $F_0^* \Omega_0 = \Phi_{\theta_0}^* \Omega_0 = \Omega_0$. Upon introducing the 2-form-valued Fourier coefficients,

$$\Omega_0^k = \frac{1}{2\pi} \int_0^{2\pi} e^{-ik\theta} \Phi_\theta^* \Omega_0 d\theta, \quad k \in \mathbb{Z}, \quad (12)$$

the last identity may be rewritten as the sequence of identities $e^{ik\theta_0} \Omega_0^k = \Omega_0^k$, $k \in \mathbb{Z}$. But by non-resonance of F , $1 - e^{ik\theta_0}$ is nonvanishing for each k . We conclude that $\Omega_0^k = 0$ for nonzero k , or, equivalently, $\mathcal{L}_{R_0} \Omega_0 = 0$.

Presymplecticity of F for nonzero γ implies $F_\gamma^* \Omega_\gamma = \Omega_\gamma$ for each $\gamma \in \Gamma$. Applying the Lie derivative \mathcal{L}_{R_γ} to this identity and using $F_\gamma^* R_\gamma = R_\gamma$ implies $F_\gamma^* (\mathcal{L}_{R_\gamma} \Omega_\gamma) = (\mathcal{L}_{R_\gamma} \Omega_\gamma)$. In other words, $\alpha_\gamma = \mathcal{L}_{R_\gamma} \Omega_\gamma$ is (formally) an absolute integral invariant for F_γ . By the argument from the previous paragraph, we see immediately that $\alpha_0 = 0$. To finish the proof, we will use integral invariance together with existence of a normalizing transformation to find that $\alpha_\gamma = 0$ to all orders in γ . This argument will parallel the proof of Proposition 3.

Let G_γ be the generator of a normalizing transformation for F given by Theorem 2. Set $\bar{\alpha}_\gamma = \exp(-\mathcal{L}_{G_\gamma})\alpha_\gamma = \bar{\alpha}_0 + \bar{\alpha}_1[\gamma] + \bar{\alpha}_2[\gamma, \gamma] + \dots$. Note that $\alpha_\gamma = 0$ if and only if $\bar{\alpha}_\gamma = 0$. Since α_γ is an integral invariant for F_γ , $\bar{\alpha}_\gamma$ must satisfy

$$\exp(-\mathcal{L}_{G_\gamma})F_\gamma^* \exp(\mathcal{L}_{G_\gamma})\bar{\alpha}_\gamma = \bar{\alpha}_\gamma. \quad (13)$$

Because $\bar{\alpha}_0 = \alpha_0 = 0$, the first-order consequence of (13) is $F_0^* \bar{\alpha}_1[\gamma] = \Phi_{\theta_0}^* \bar{\alpha}_1[\gamma] = \bar{\alpha}_1[\gamma]$. By our earlier argument, we must then have $(\bar{\alpha}_1[\gamma])^k = 0$ for $k \neq 0$. But using $\exp(-\mathcal{L}_{G_\gamma})R_\gamma = R_0$, we also find $\bar{\alpha}_\gamma = \mathcal{L}_{R_0} \bar{\Omega}_\gamma$, where $\bar{\Omega}_\gamma = \exp(-\mathcal{L}_{G_\gamma})\Omega_\gamma$. The latter implies $\bar{\alpha}_\gamma^0 = 0$, and $(\bar{\alpha}_1[\gamma])^0 = 0$ in particular. Thus, $\bar{\alpha}_1[\gamma] = 0$ for all $\gamma \in \Gamma$. We may now repeat this argument for $\bar{\alpha}_2[\gamma, \gamma]$, $\bar{\alpha}_3[\gamma, \gamma, \gamma]$, etc., to obtain the desired result. \square

Using presymplecticity of the roto-rate, we may now use a version of Noether's theorem to establish existence of adiabatic invariants for many interesting presymplectic nearly periodic maps.

Theorem 4 (Existence of an adiabatic invariant) *Let F be a non-resonant presymplectic nearly periodic map on the exact γ -dependent presymplectic manifold (M, Ω_γ) with roto-rate R_γ . Assume one of the following conditions is satisfied.*

- (1) F is Hamiltonian.
- (2) M is connected and the limiting roto-rate R_0 has at least one zero.

There exists a smooth γ -dependent 1-form θ_γ such that $\mathcal{L}_{R_\gamma} \theta_\gamma = 0$ and $-\mathbf{d}\theta_\gamma = \Omega_\gamma$ in the sense of formal power series. Moreover the quantity

$$\mu_\gamma = \iota_{R_\gamma} \theta_\gamma \quad (14)$$

satisfies $F_\gamma^ \mu_\gamma = \mu_\gamma$ in the sense of formal power series. In other words, μ_γ is an adiabatic invariant for F .*

Proof By Theorem 3, a primitive θ_γ with the desired properties may be constructed as in the proof of Proposition 4.

To establish adiabatic invariance of μ_γ , first we compute the exterior derivative of μ_γ using Cartan's formula to obtain $\mathbf{d}\mu_\gamma = \iota_{R_\gamma} \Omega_\gamma$. Since both R_γ and Ω_γ are F_γ -invariant, it follows that $\mathbf{d}F_\gamma^* \mu_\gamma = \mathbf{d}\mu_\gamma$. The difference $c_\gamma \equiv F_\gamma^* \mu_\gamma - \mu_\gamma$ must therefore be a formal power series whose coefficients are homogeneous polynomial maps from Γ into locally constant functions on M . To complete the proof, we must demonstrate that $c_\gamma = 0$ to all orders.

First suppose F is Hamiltonian. Then, there is a smooth (t, γ) -dependent Hamiltonian vector field $Y_{t,\gamma}$ with Hamiltonian $H_{t,\gamma}$ whose $t = 1$ flow is equal to F_γ . Let \mathcal{F}_t^γ denote the time- t flow map for $Y_{t,\gamma}$ with $\mathcal{F}_0^\gamma = \text{id}_M$. By the fundamental theorem of calculus, the definition of Lie derivative, and Cartan's formula, we therefore have

$$\begin{aligned} F_\gamma^* \mu_\gamma &= \iota_{R_\gamma} (\mathcal{F}_1^\gamma)^* \theta_\gamma \\ &= \iota_{R_\gamma} \theta_\gamma + \iota_{R_\gamma} \int_0^1 \frac{d}{dt} (\mathcal{F}_t^\gamma)^* \theta_\gamma dt \\ &= \mu_\gamma + \iota_{R_\gamma} \int_0^1 (\mathcal{F}_t^\gamma)^* (\mathcal{L}_{Y_{t,\gamma}} \theta_\gamma) dt \\ &= \mu_\gamma + \iota_{R_\gamma} \int_0^1 (\mathcal{F}_t^\gamma)^* (\iota_{Y_{t,\gamma}} \mathbf{d}\theta_\gamma + \mathbf{d}\iota_{Y_{t,\gamma}} \theta_\gamma) dt \\ &= \mu_\gamma + \iota_{R_\gamma} \int_0^1 (\mathcal{F}_t^\gamma)^* \mathbf{d}(\iota_{Y_{t,\gamma}} \theta_\gamma - H_{t,\gamma}) dt \\ &= \mu_\gamma + \mathcal{L}_{R_\gamma} \int_0^1 (\mathcal{F}_t^\gamma)^* (\iota_{Y_{t,\gamma}} \theta_\gamma - H_{t,\gamma}) dt. \end{aligned}$$

Applying $\exp(\theta \mathcal{L}_{R_0})$ to this identity and averaging in θ gives the desired result.

Finally suppose that M is connected and that $R_0(m_0) = 0$ for some $m_0 \in M$. Let G_γ be the generator of a normalizing transformation. We have

$$\exp(-\mathcal{L}_{G_\gamma}) \mu_\gamma(m_0) = \iota_{R_0} \exp(-\mathcal{L}_{G_\gamma}) \theta_\gamma(m_0) = 0,$$

and

$$\exp(-\mathcal{L}_{G_\gamma}) F_\gamma^* \mu_\gamma(m_0) = \exp(-\mathcal{L}_{G_\gamma}) \iota_{R_\gamma} F_\gamma^* \theta_\gamma(m_0) = \iota_{R_0} (\exp(-\mathcal{L}_{G_\gamma}) F_\gamma^* \theta_\gamma)(m_0) = 0.$$

It follows that c_γ is zero on the connected component of M containing m_0 . But since M is connected, c_γ is therefore zero everywhere, as claimed. \square

Remark 3 A simple example illustrates how existence of an adiabatic invariant can fail. Let $M = S^1 \times \mathbb{R} \ni (\zeta, I)$, $\Omega_\gamma = d\zeta \wedge dI = -\mathbf{d}(I d\zeta)$, and $\Gamma = \mathbb{R}$. The mapping $F(\zeta, I, \gamma) = (\zeta + \theta_0, I + \gamma)$ defines a non-resonant nearly periodic map for almost all $\theta_0 \in U(1)$. The roto-rate is given to all orders by $R_\gamma = \partial_\zeta$. Moreover, F_γ is area-preserving for each γ , and hence presymplectic. The quantity $\mu_\gamma = \iota_{R_\gamma} (I d\zeta) = I$ from (14) is clearly not an adiabatic invariant for F since $F_\gamma^* I = I + \gamma$. Note that, in this example, the R_0 -orbits are not contractible and that F is presymplectic but not Hamiltonian.

4.2 Geometric Integration of Noncanonical Hamiltonian Systems Using Nearly Periodic Maps

Let $Q \subset E$ be a connected open subset of a finite-dimensional vector space E equipped with an exact symplectic form $\omega = -\mathbf{d}\vartheta$. Consider a Hamiltonian system on $(Q, \omega = -\mathbf{d}\vartheta)$ with Hamiltonian $H : Q \rightarrow \mathbb{R}$. Choose an almost complex structure $\mathbb{J} : TQ \rightarrow TQ$ compatible with the symplectic form $\omega = -\mathbf{d}\vartheta$, so that $g(v, w) = \omega(v, \mathbb{J}w)$

defines a metric tensor on Q . Equip the tangent bundle $\pi : TQ \rightarrow Q$ with the “magnetic” symplectic form

$$\Omega_\epsilon^* = \pi^* \omega + \epsilon \Omega,$$

where ϵ is a real parameter and Ω is the pullback of the canonical symplectic form on T^*Q along the bundle map $TQ \rightarrow T^*Q$ defined by g . We may also define a natural Hamilton function on TQ ,

$$H_\epsilon^*(q, v) = \frac{1}{2} \epsilon^2 g_q(v, v) + \epsilon H(q).$$

As explained in detail in Burby and Hirvijoki (2021), H_ϵ^* defines a Hamiltonian nearly periodic system whose slow manifold dynamics recovers the dynamics of H on Q as $\epsilon \rightarrow 0$. The limiting roto-rate is

$$R_0(q, v) = \mathbb{J}_q(v - X_H(q)) \cdot \partial_v, \quad (15)$$

where X_H denotes the Hamiltonian vector field on Q associated with H , and the angular frequency function $\omega_0 = 1$. Moreover, the adiabatic invariant associated with H_ϵ^* ensures that the slow manifold enjoys long-term normal stability. It is crucial that the metric g is determined by an almost complex structure \mathbb{J} compatible with ω for these results to hold. If g is a more general metric tensor then the larger system on TQ need not be nearly periodic, and an adiabatic invariant need not exist.

The purpose of this section is to combine observations from Burby and Hirvijoki (2021) with the theory of nearly periodic maps in order to construct a geometric numerical integrator for H . The integrator will be given as an implicitly defined mapping on TQ that is provably presymplectic nearly periodic with limiting roto-rate R_0 . We will show that this mapping admits a slow manifold diffeomorphic to Q on which iterations of the map approximate the H -flow. In fact, the mapping is a slow manifold integrator in the sense described in Burby and Klotz (2020). In addition, we will argue using the Noether theorem for nearly periodic maps that this discrete-time slow manifold enjoys long-term normal stability. This ensures that the mapping on TQ will function effectively and reliably as a structure-preserving integrator for the original Hamiltonian system on Q . We remark that the results described in this section provide a general solution to the problem of structure-preserving integration of non-canonical Hamiltonian systems on exact symplectic manifolds. For a completely different approach that is less geometric, we refer readers to Kraus (2017).

We begin with some preliminary remarks.

Remark 4 It will be convenient to work with the parameter $\hbar = \sqrt{\epsilon}$ instead of ϵ . There are technical reasons for doing so that will not be discussed here; however, an obvious physical benefit will be that \hbar may be interpreted as a timestep. The symplectic form on TQ will therefore be given by

$$\Omega_\hbar^* = \pi^* \omega + \hbar^2 \Omega.$$

Remark 5 It is useful to describe the goal of our construction in more concrete terms. We aim to find a smooth \hbar -dependent mapping $\Psi_{\hbar} : TQ \rightarrow TQ$ that is both non-resonant nearly periodic with limiting roto-rate R_0 given by (15) and symplectic, $\Psi_{\hbar}^* \Omega_{\hbar}^* = \Omega_{\hbar}^*$, for all $\hbar \ll 1$. Since Q is connected and R_0 has a manifold of fixed points of the form $\{(q, X_H(q))\} \subset TQ$, Theorem 4 (Noether's theorem for nearly periodic maps) ensures that the mapping we seek will admit an adiabatic invariant μ_{\hbar} .

Remark 6 We may determine the leading-order term in the formal power series $\mu_{\hbar} = \mu_0 + \hbar \mu_1 + \hbar^2 \mu_2 + \dots$ using only the explicit expressions for Ω_{\hbar}^* and R_0 in conjunction with the general existence theorem (Theorem 4). Recall that the theorem says that the adiabatic invariant is given by $\mu_{\hbar} = \iota_{R_{\hbar}} \overline{\Theta}_{\hbar}$, where R_{\hbar} is the roto-rate and $\overline{\Theta}_{\hbar}$ is a $U(1)$ -invariant primitive for Ω_{\hbar}^* . In particular, the roto-rate must satisfy Hamilton's equation $\iota_{R_{\hbar}} \Omega_{\hbar}^* = \mathbf{d}\mu_{\hbar}$ with Hamiltonian μ_{\hbar} . We apply this theorem as follows.

If $f : TQ \rightarrow \mathbb{R}$ is any smooth \hbar -independent function on TQ then it is straightforward to verify that $X_f = \hbar^{-4}(\mathbb{J} \partial_v f) \cdot \partial_v + \text{l.o.t.}$. Therefore, we must have $R_{\hbar} = \hbar^{-4}(\mathbb{J} \partial_v \mu_0) \cdot \partial_v + \text{l.o.t.}$. But since $R_{\hbar} = O(1)$, the last expression implies $\partial_v \mu_0 = 0$ everywhere on TQ , or $\mu_0 = \mu_0(q)$. In fact $\mu_0(q)$ must be constant, for if $(q, v_{\hbar}(q))$ is a zero for R_{\hbar} then Hamilton's equation implies $0 = \lim_{\hbar \rightarrow 0} \mathbf{d}\mu_{\hbar}(q, v_{\hbar}(q)) = \mathbf{d}\mu_0(q)$. And by evaluating the formula $\mu_{\hbar} = \iota_{R_{\hbar}} \overline{\Theta}_{\hbar}$ at $(q, v_{\hbar}(q))$ we find that the constant must in fact be 0. In other words $\mu_0 = 0$. Essentially, the same argument may now be applied to conclude $\mu_1 = \mu_2 = \mu_3 = 0$; the argument for μ_1 proceeds as follows. Since $\mu_0 = 0$, Hamilton's equation implies $R_0 = \hbar^{-3}(\mathbb{J} \partial_v \mu_1) \cdot \partial_v + \text{l.o.t.}$, or $\mu_1 = \mu_1(q)$. Evaluating Hamilton's equation at $(q, v_{\hbar}(q))$, dividing by \hbar , and taking the limit $\hbar \rightarrow 0$ then leads to $0 = \lim_{\hbar \rightarrow 0} \hbar^{-1} \mathbf{d}\mu_{\hbar}(q, v_{\hbar}(q)) = \mathbf{d}\mu_1(q)$, implying μ_1 is a constant. Applying the same procedure to the formula $\mu_{\hbar} = \iota_{R_{\hbar}} \overline{\Theta}_{\hbar}$ implies the constant must be 0.

We have now established that the adiabatic invariant for the nearly periodic map we aim to construct must have the form $\mu_{\hbar} = \hbar^4 \mu_4 + \hbar^5 \mu_5 + \dots$. We can determine an explicit expression for μ_4 as follows. By the above remarks, we must have $R_{\hbar} = (\mathbb{J} \partial_v \mu_4) \cdot \partial_v + \text{l.o.t.}$, which implies in particular that $R_0 = (\mathbb{J} \partial_v \mu_4) \cdot \partial_v$. Since the desired form of R_0 is known, we therefore obtain the following partial differential equation for μ_4 :

$$\mathbb{J}(v - X_H) = \mathbb{J} \partial_v \mu_4.$$

The general solution of this equation is given by $\mu_4(q, v) = \frac{1}{2} g_q(v - X_H(q), v - X_H(q)) + \chi(q)$, where $\chi(q)$ is an arbitrary function of q . To determine χ , we evaluate the formula $\mu_{\hbar} = \iota_{R_{\hbar}} \overline{\Theta}_{\hbar}$ at a fixed point $(q, v_{\hbar}(q))$ to find $0 = \lim_{\hbar \rightarrow 0} \hbar^{-4} \mu_{\hbar}(q, v_{\hbar}(q)) = \mu_4(q, v_0(q)) = \chi(q)$. Note that we have used the formula for $v_0(q) = X_H(q)$ for fixed points of R_0 . We conclude that the adiabatic invariant must have the general form

$$\mu_{\hbar}(q, v) = \hbar^4 \frac{1}{2} g_q(v - X_H(q), v - X_H(q)) + O(\hbar^5). \quad (16)$$

This formula will be useful later when we argue for long-term normal stability.

To construct the mapping $\Psi_{\hbar} : TQ \rightarrow TQ$, we begin by introducing the mixed-variable generating function

$$S : Q \times Q \rightarrow \mathbb{R}$$

$$S(q, \bar{q}) = \int_q^{\bar{q}} \vartheta + \Phi^* \Sigma(q, \bar{q}), \quad (17)$$

where $\Phi(q, \bar{q}) = (q/2 + \bar{q}/2, \bar{q} - q)$ is a diffeomorphism $Q \times Q \rightarrow TQ$, and $\Sigma : TQ \rightarrow \mathbb{R}$ is given by

$$\Sigma(x, \xi) = -\hbar H(x) + \hbar^2 \langle X_H(x), \xi \rangle - \frac{1}{12} \hbar^2 \partial_k \omega_{j\ell}(x) X_H^k(x) X_H^j(x) \xi^\ell$$

$$- \frac{1}{4} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) \langle \xi - \hbar X_H(x), \xi - \hbar X_H(x) \rangle.$$

Here, $\langle \cdot, \cdot \rangle$ is shorthand for $g(\cdot, \cdot)$, the integral is taken along the straight line connecting q with \bar{q} , $X_H = -\mathbb{J} \nabla H$ is the Hamiltonian vector field associated with H , and $\theta_0 \notin \{0, \pi\}$. The metric tensor, the Hamiltonian, and the Hamiltonian vector field are evaluated at the midpoint $x = (\bar{q} + q)/2$. The variables q and \bar{q} should be interpreted as the “old” and “new” points in the symplectic manifold Q . While it is not necessary to go into the details here, the function S may be understood as an approximation of Jacobi’s solution of the Hamilton Jacobi equation for the Hamiltonian H_ϵ^* .

Definition 14 The **symplectic Lorentz map** is the mapping $\Psi_{\hbar} : TQ \rightarrow TQ : (q, v) \mapsto (\bar{q}, \bar{v})$ defined by the implicit relations

$$\vartheta_{\bar{q}} + \hbar^2 g_{\bar{q}}(\bar{v}, d\bar{q}) = \mathbf{d}^{(2)} S, \quad (18)$$

$$\vartheta_q + \hbar^2 g_q(v, dq) = -\mathbf{d}^{(1)} S. \quad (19)$$

Here $g_{\bar{q}}(\bar{v}, d\bar{q})$ is the linear map $T_{\bar{q}}Q \rightarrow \mathbb{R}$ given by $\bar{w}_{\bar{q}} \mapsto g_{\bar{q}}(\bar{v}, \bar{w}_{\bar{q}})$, and $g_q(v, dq)$ is defined analogously.

Proposition 5 *The symplectic Lorentz map is well-defined and smooth in (q, v, \hbar) for \hbar in a neighborhood of $0 \in \mathbb{R}$. Moreover, it preserves the \hbar -dependent symplectic form Ω_{\hbar}^* and satisfies*

$$\Psi_0(q, v) = (x, X_H(q) + \exp(-\theta_0 \mathbb{J}(q))[v - X_H(q)]). \quad (20)$$

Proof First we will construct a convenient moving frame on $Q \times Q$ onto which we will resolve the implicit relations (18) and (19). We will start by building a frame on TQ and then finish by pulling back along the mapping $\Phi : Q \times Q \rightarrow TQ$ defined above. Without loss of generality, assume $Q = \mathbb{R}^n$ for an even integer n and let (x^i, ξ^i) denote the standard linear coordinate system on TQ . Fix $(x, \xi) \in TQ$ and let $\gamma : [-1, 1] \rightarrow Q$ be a smooth curve in Q with $\gamma(0) = x$. Relative to the Riemannian structure defined by the metric g there is a unique horizontal lift

$\tilde{\gamma} : [-1, 1] \rightarrow TQ$ with $\tilde{\gamma}(0) = (x, \xi)$. In this manner, to each $(x, \xi) \in TQ$ and each tangent vector $w \in T_x Q$ we assign a lifted tangent vector $\tilde{w} \in T_{(x, \xi)} TQ$. Applying this construction point-wise to the coordinate vector fields ∂_{x^i} on Q , we obtain linearly independent vector fields $\tilde{\partial}_{x^i}$ on TQ . The collection of $2n$ vector fields $(\tilde{\partial}_{x^i}, \partial_{\xi^i})$ comprise a frame on TQ . A frame on $Q \times Q$ is then furnished by the vector fields (U^i, A^i) , where $U^i = \Phi^* \tilde{\partial}_{x^i}$ and $A^i = \Phi^* \partial_{\xi^i}$. Upon introducing the Christoffel symbols $\nabla_{\partial_{x^i}} \partial_{x^j} = \Gamma_{ij}^k \partial_{x^k}$, the vector fields $\tilde{\partial}_{x^i}$ may be written as

$$\tilde{\partial}_{x^i} = \partial_{x^i} - \Gamma_{ij}^k(x) \xi^j \partial_{\xi^k}.$$

Therefore, we may write the following explicit formulas for the frame (U^i, A^i) :

$$\begin{aligned} U^i &= \left(\partial_{q^i} + \frac{1}{2} \Gamma_{ij}^k(x) \xi^j \partial_{q^k} \right) + \left(\partial_{\bar{q}^i} - \frac{1}{2} \Gamma_{ij}^k(x) \xi^j \partial_{\bar{q}^k} \right) \\ A^i &= -\frac{1}{2} \partial_{q^i} + \frac{1}{2} \partial_{\bar{q}^i}, \end{aligned}$$

where we remind the reader that $x = (q + \bar{q})/2$ and $\xi = \bar{q} - q$.

Next, we rewrite (18) and (19) as a single equation on $Q \times Q$,

$$\vartheta_{\bar{q}}(d\bar{q}) - \vartheta_q(dq) + \hbar^2 g_{\bar{q}}(\bar{v}, d\bar{q}) - \hbar^2 g_q(v, dq) = \mathbf{dS}, \quad (21)$$

and then take components along the frame (U^i, A^i) to obtain

$$\begin{aligned} &\hbar^2 g_{\ell i}(\bar{q}) \bar{v}^\ell - \hbar^2 g_{\ell i}(q) v^\ell - \frac{1}{2} \hbar^2 \Gamma_{ij}^k(x) \xi^j \left(g_{\ell k}(\bar{q}) \bar{v}^\ell + g_{\ell k}(q) v^\ell \right) \\ &= \int_0^1 \xi^j \omega_{ji}(\lambda) d\lambda - \int_0^1 \left[\lambda - \frac{1}{2} \right] \xi^j \omega_{jk}(\lambda) \Gamma_{i\ell}^k(x) \xi^\ell d\lambda \\ &\quad - \hbar \partial_i H(x) + \frac{\hbar}{2} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) g_{\ell j}(x) X_{H;i}^\ell(x) (\xi^j - \hbar X_H^j(x)) \\ &\quad - \frac{1}{12} \hbar^2 \partial_i (\partial_k \omega_{j\ell} X_H^k X_H^j) \xi^\ell + \frac{1}{12} \hbar^2 \partial_k \omega_{j\ell} X_H^k X_H^j \Gamma_{im}^\ell \xi^m, \end{aligned}$$

and

$$\begin{aligned} &\frac{1}{2} \hbar^2 g_{\ell i}(\bar{q}) \bar{v}^\ell + \frac{1}{2} \hbar^2 g_{\ell i}(q) v^\ell \\ &= \int_0^1 \left[\lambda - \frac{1}{2} \right] \xi^j \omega_{ji}(\lambda) d\lambda - \frac{1}{12} \hbar^2 \partial_k \omega_{ji} X_H^k X_H^j \\ &\quad + \hbar^2 g_{ij}(x) X_H^j(x) - \frac{1}{2} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) g_{ij}(x) (\xi^j - \hbar X_H^j(x)). \end{aligned}$$

Here, we have applied the useful formulas

$$\mathbf{d} \int_q^{\bar{q}} \vartheta = \vartheta_{\bar{q}}(d\bar{q}) - \vartheta_q(dq) + \int_0^1 \omega_\lambda(\xi, [1 - \lambda]dq + \lambda d\bar{q}) d\lambda$$

and

$$\begin{aligned} \mathcal{L}_{\tilde{q}_{x^i}} \Sigma &= -\hbar \partial_i H + \frac{\hbar}{2} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) g(\nabla_{\partial_i} X_H, \xi - \hbar X_H) \\ &\quad - \frac{1}{12} \hbar^2 \partial_i (\partial_k \omega_{j\ell} X_H^k X_H^j) \xi^\ell + \frac{1}{12} \hbar^2 \partial_k \omega_{j\ell} X_H^k X_H^j \Gamma_{im}^\ell \xi^m \\ \mathcal{L}_{\partial_{\xi^i}} \Sigma &= \hbar^2 g(X_H, \partial_{x^i}) - \frac{1}{12} \hbar^2 \partial_k \omega_{ji} X_H^k X_H^j - \frac{1}{2} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) g(\xi - \hbar X_H, \partial_{x^i}), \end{aligned}$$

where $\omega_\lambda = \omega_{q(\lambda)}$ with $q(\lambda) = [1 - \lambda]q + \lambda \bar{q}$.

To show that these implicit equations define a smooth \hbar -dependent mapping Ψ_\hbar , we first introduce the new variable $\Delta = \hbar^{-2}(\xi - \hbar X_H(x))$ and then observe that when expressed in terms of Δ the implicit equations above may be written in the form

$$\hbar^2 g_{\ell i}(x) (\bar{v}^\ell - v^\ell) = \hbar^2 \Delta^j \omega_{ji}(x) + O(\hbar^3)$$

and

$$\frac{1}{2} \hbar^2 g_{\ell i}(x) (\bar{v}^\ell + v^\ell) = \hbar^2 g_{ij}(x) X_H^j(x) - \hbar^2 \frac{1}{2} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) g_{ij}(x) \Delta^j + O(\hbar^3).$$

Note in particular that the term $\frac{1}{12} \hbar^2 \partial_k \omega_{ji} X_H^k X_H^j$ exactly cancels the second-order part of $\int_0^1 [\lambda - \frac{1}{2}] \xi^j \omega_{ji}(\lambda) d\lambda$. Dividing these expressions by \hbar^2 implies that there are smooth functions $Z_1, Z_2 : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}^n$ given by

$$\begin{aligned} Z_{1i}(x, v, \Delta, \bar{v}, \hbar) &= g_{\ell i}(x) (\bar{v}^\ell - v^\ell) - \Delta^j \omega_{ji}(x) + O(\hbar), \\ Z_{2i}(x, v, \Delta, \bar{v}, \hbar) &= \frac{1}{2} g_{\ell i}(x) (\bar{v}^\ell + v^\ell) - g_{ij}(x) X_H^j(x) \\ &\quad + \frac{1}{2} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) g_{ij}(x) \Delta^j + O(\hbar), \end{aligned}$$

such that the implicit equations defining the symplectic Lorentz map are satisfied if and only if

$$Z_1(x, v, \Delta, \bar{v}, \hbar) = Z_2(x, v, \Delta, \bar{v}, \hbar) = 0.$$

When $\hbar = 0$, the unique solution of these equations for Δ and \bar{v} is

$$\begin{aligned} \Delta_0 &= (1 - \exp(-\theta_0 \mathbb{J})) \mathbb{J} (v - X_H(x)), \\ \bar{v}_0 &= X_H(x) - \exp(-\theta_0 \mathbb{J}) [v - X_H(x)]. \end{aligned}$$

Moreover, for each (x, v) , the (Δ, \bar{v}) derivative of $(Z_1, Z_2)^T$ at $(x, v, \Delta_0, \bar{v}_0, 0)$ is given by

$$\begin{pmatrix} D_{\Delta} Z_1(x, v, \Delta_0, \bar{v}_0) & D_{\bar{v}} Z_1(x, v, \Delta_0, \bar{v}_0) \\ D_{\Delta} Z_2(x, v, \Delta_0, \bar{v}_0) & D_{\bar{v}} Z_2(x, v, \Delta_0, \bar{v}_0) \end{pmatrix} = \begin{pmatrix} -\mathbb{J}(x) & 1 \\ \frac{1}{2} \begin{pmatrix} \sin \theta_0 \\ 1 - \cos \theta_0 \end{pmatrix} & \frac{1}{2} \end{pmatrix},$$

which is invertible. The implicit function theorem therefore implies there is a unique pair of smooth functions $\Delta(x, v, \hbar), \bar{v}(x, v, \hbar)$ defined in an open neighborhood of $\{(x, v, \hbar) \mid \hbar = 0\} \subset \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}$ that satisfy the equations

$$Z_1(x, v, \Delta(x, v, \hbar), \bar{v}(x, v, \hbar)) = Z_2(x, v, \Delta(x, v, \hbar), \bar{v}(x, v, \hbar)) = 0.$$

Since Δ is related to \bar{q} by

$$\bar{q} = x + \frac{1}{2} \hbar X_H(x) + \frac{1}{2} \hbar^2 \Delta(x, v, \hbar),$$

another simple application of the implicit function theorem establishes existence and smoothness of the symplectic Lorentz map $\Psi_{\hbar} : (q, v) \mapsto (\bar{q}, \bar{v})$. We have also shown that Ψ_0 has the desired form $(q, v) \mapsto (q, \bar{v}_0)$. Symplecticity of Ψ_{\hbar} now follows immediately from applying the exterior derivative to (21). \square

Corollary 2 *The symplectic Lorentz map is a presymplectic nearly periodic map. It is non-resonant provided $\theta_0/2\pi \notin \mathbb{Q}$.*

We have thus constructed a nearly periodic map with the desired roto-rate and integral invariant. Now we must establish the precise sense in which the symplectic Lorentz map Ψ_{\hbar} , which is *a priori* a mapping $TQ \rightarrow TQ$, functions as a consistent numerical integrator for the Hamiltonian system X_H on Q . The first hint as to how this might work is that the limit map Ψ_0 admits a manifold of fixed points given by $\Gamma_0 = \{(x, v) \in TQ \mid v = X_H(q)\}$. This limiting invariant manifold, being the graph of X_H , is manifestly diffeomorphic to Q . Thus, if Γ_0 can be continued to an invariant manifold Γ_{\hbar} for Ψ_{\hbar} with $\hbar \neq 0$, we would automatically obtain dynamics on Q that could be compared with those of X_H by restricting Ψ_{\hbar} to Γ_{\hbar} .

Unfortunately, Γ_0 is unlikely to continue as a true invariant manifold since each fixed point on Γ_0 is of elliptic type. Instead, we can obtain the following weaker result. Roughly speaking, it says that there is a unique invariant continuation of Γ_0 at the level of formal power series in \hbar .

Proposition 6 *Denote the components of the symplectic Lorentz map as $\Psi_{\hbar} = (\Psi_{\hbar}^q, \Psi_{\hbar}^v) : (q, v) \mapsto (\bar{q}, \bar{v})$. Assume $\theta_0 \neq 0 \bmod 2\pi$. There exists a formal power series*

$$v_{\hbar}^*(q) = X_H(q) + \hbar v_1^*(q) + \hbar^2 v_2^*(q) + \dots$$

with vector field coefficients such that

$$\Psi_{\hbar}^v(q, v_{\hbar}^*(q)) = v_{\hbar}^*(\Psi_{\hbar}^q(q)), \quad (22)$$

where

$$\psi_h(q) = \Psi_h^q(q, v_h^*(q)).$$

Proof Expanding the condition (22) in powers of \hbar leads to an infinite sequence of constraints that the formal power series v_h^* must obey. Simultaneous satisfaction of each constraint in the sequence is equivalent to (22). The first two constraints are given explicitly by

$$\begin{aligned}\Psi_0^v(q, X_H(q)) &= X_H(q), \\ \Psi_1^v(q, X_H(q)) + D_v \Psi_0^v(q, X_H(q))[v_1^*(q)] &= v_1^*(q) + DX_H(q)[\Psi_1^q(q, X_H(q))],\end{aligned}$$

where we have introduced the formal series expansions

$$\Psi_h^q = \Psi_0^q + \hbar \Psi_1^q + \dots, \quad \Psi_h^v = \Psi_0^v + \hbar \Psi_1^v + \dots$$

and used $\Psi_0^q(q, v) = q$. Glancing at (20) reveals that the first of these equations is automatically satisfied. The second equation can be interpreted as an algebraic equation constraining the form of v_1^* . In fact, since the linear map

$$\begin{aligned}L(q) &= D_v \Psi_0^v(q, X_H(q)) - \text{id}, \\ \delta v &\mapsto \exp(-\theta_0 \mathbb{J}(q))[\delta v] - \delta v,\end{aligned}$$

is invertible whenever $\theta_0 \neq 0 \bmod 2\pi$, v_1^* is determined uniquely by the formula

$$v_1^*(q) = L(q)^{-1}[DX_H(q)[\Psi_1^q(q, X_H(q))] - \Psi_1^v(q, X_H(q))].$$

More generally, the n^{th} equation in the sequence has the form

$$L(q)[v_n^*(q)] = s_n(q),$$

where $s_n(q)$ depends only on coefficients of the power series expansion for Ψ_h and coefficients v_k^* with $k < n$. Invertibility of $L(q)$ therefore implies that there is a unique formula for v_n^* for each n . The formal power series v_h^* defined in this manner satisfies (22) by construction. \square

So while we do not obtain a genuine invariant manifold diffeomorphic to \mathcal{Q} , we do obtain a family of approximate invariant manifolds diffeomorphic to \mathcal{Q} given by truncations of the formal power series v_h^* . Using arguments comparable to those presented in Burby and Hirvijoki (2021), it is possible to show that truncations of v_h^* may be constructed so their graphs agree with the zero level set of the adiabatic invariant μ_h for Ψ_h to any desired order in \hbar . Adiabatic invariance of μ_h can then be used to prove the existence of manifolds $\Gamma_h^{(n)}$ close to Γ_0 with the following schematic normal stability property:

- For each $N > 0$ and (q, v) within $\hbar^{\alpha(n)}$ of $\Gamma_{\hbar}^{(n)}$ the point $\Psi_{\hbar}^k(q, v)$ remains within $\hbar^{\beta(n)}$ of $\Gamma_{\hbar}^{(n)}$ for $k = O(\epsilon^{-N})$. Here α and β are monotone increasing functions of n .

We will not attempt to prove such a result in full generality here. However, since we have already determined the form of the leading term in the adiabatic invariant series (in this case $\mu_{\hbar} = \hbar^4 \mu_4 + O(\hbar^5)$), we can prove a special case of the general result without much effort. First we establish the timescale over which μ_4 is well-conserved.

Definition 15 Given a compact set $C \subset TQ$, a point (q, v) is **positively contained** if $\Psi_{\hbar}^k(q, v) \in C$ for all nonnegative integers k and all \hbar in a neighborhood of 0.

Proposition 7 For each $N > 0$ and compact set $C \subset TQ$ there is a positive, \hbar -independent constant \mathcal{M} such that

$$|\mu_4(\Psi_{\hbar}^k(q, v)) - \mu_4(q, v)| \leq \mathcal{M} \hbar, \quad k \in [0, k^*(\hbar, N)],$$

whenever (q, v) is positively contained in C . Here $k^*(\hbar, N) = O(\hbar^{-N})$.

Proof First we will obtain a useful estimate for the degree of conservation of an arbitrary truncation of the adiabatic invariant series. Let $\bar{\mu}_{\hbar} = \hbar^{-4} \mu_{\hbar} = \mu_4 + \hbar \mu_5 + \dots$ denote the reduced adiabatic invariant for the symplectic Lorentz map. Define $\bar{\mu}_i = \mu_{i+4}$ and let $\bar{\mu}_{\hbar}^{(N)} = \sum_{i=0}^N \bar{\mu}_i \hbar^i$. Since $\bar{\mu}_{\hbar}^{(N)} = \bar{\mu}_{\hbar} + O(\hbar^{N+1})$ and $\bar{\mu}_{\hbar}$ is Ψ_{\hbar} -invariant to all orders in \hbar , there is a constant \mathcal{M}_N , depending on both C and N , such that

$$\forall (q, v) \in C, |\bar{\mu}_{\hbar}^{(N)}(\Psi_{\hbar}(q, v)) - \bar{\mu}_{\hbar}^{(N)}(q, v)| \leq \mathcal{M}_N \hbar^{N+1}.$$

For positively contained (q, v) , we may apply this formula repeatedly to obtain an estimate for the change in $\bar{\mu}_{\hbar}^{(N)}$ after k positive timesteps,

$$\begin{aligned} |\bar{\mu}_{\hbar}^{(N)}(\Psi_{\hbar}^k(q, v)) - \bar{\mu}_{\hbar}^{(N)}(q, v)| &\leq \mathcal{M}_N \hbar^{N+1} + |\bar{\mu}_{\hbar}^{(N)}(\Psi_{\hbar}^{k-1}(q, v)) - \bar{\mu}_{\hbar}^{(N)}(q, v)| \\ &\leq (1+k)\mathcal{M}_N \hbar^{N+1}. \end{aligned} \quad (23)$$

Next, we draw implications from the previous inequality together with a bound on the difference between $\bar{\mu}_{\hbar}^{(0)} = \mu_4$ and $\bar{\mu}_{\hbar}^{(N)}$. There must be another positive constant \mathcal{M}'_N , depending on both C and N , such that

$$\forall (q, v) \in C, |\bar{\mu}_{\hbar}^{(0)}(q, v) - \bar{\mu}_{\hbar}^{(N)}(q, v)| \leq \mathcal{M}'_N \hbar.$$

In light of the inequality (23), this implies that for each positively contained (q, v) the change in $\bar{\mu}_{\hbar}^{(0)}$ after k positive timesteps is at most

$$\begin{aligned} &|\bar{\mu}_{\hbar}^{(0)}(\Psi_{\hbar}^k(q, v)) - \bar{\mu}_{\hbar}^{(0)}(q, v)| \\ &\leq |\bar{\mu}_{\hbar}^{(0)}(\Psi_{\hbar}^k(q, v)) - \bar{\mu}_{\hbar}^{(N)}(\Psi_{\hbar}^k(q, v))| + |\bar{\mu}_{\hbar}^{(N)}(\Psi_{\hbar}^k(q, v)) - \bar{\mu}_{\hbar}^{(0)}(q, v)| \end{aligned}$$

$$\begin{aligned}
&\leq \mathcal{M}'_N \hbar + |\bar{\mu}_\hbar^{(N)}(\Psi_\hbar^k(q, v)) - \bar{\mu}_\hbar^{(0)}(q, v)| \\
&\leq \mathcal{M}'_N \hbar + |\bar{\mu}_\hbar^{(N)}(\Psi_\hbar^k(q, v)) - \bar{\mu}_\hbar^{(N)}(q, v)| \\
&\quad + |\bar{\mu}_\hbar^{(N)}(q, v) - \bar{\mu}_\hbar^{(0)}(q, v)| \\
&\leq 2\mathcal{M}'_N \hbar + (1 + k)\mathcal{M}_N \hbar^{N+1}.
\end{aligned}$$

Apparently, the change in $\mu_4 = \bar{\mu}_\hbar^{(0)}$ is at most $O(\hbar)$ as long as $k \hbar^{N+1} = O(\hbar)$. We therefore obtain the desired inequality with $k^*(\hbar, N) = \lfloor \hbar^{-N} \rfloor - 1$. \square

Remark 7 If “positively contained” fails, then the next best thing would be having uniform bounds (in TQ and \hbar) on the derivatives of Ψ_\hbar . The precise form of these bounds would depend on the details of the underlying Hamiltonian system on Q . Then, the proof of the previous proposition would go through practically unchanged. In the absence of both positively containment and uniform boundedness, things get trickier, and we have no general answer as to the validity of Proposition 7.

Using this result together with the explicit form of μ_4 , we now easily obtain the following normal stability result for the almost invariant set given by the graph of X_H .

Proposition 8 *Let $C \subset TQ$ be a compact set and set $(q^k, v^k) = \Psi_\hbar^k(q, v)$ for any $(q, v) \in TQ$. Let $|\cdot|$ denote the velocity norm provided by the metric tensor g . For each $N > 0$, $V_0 > 0$, and positively contained $(q, v) \in C$ that satisfies*

$$|v - X_H(q)|_q < V_0 \sqrt{\hbar},$$

there is a positive constant V_1 such that

$$|v^k - X_H(q^k)|_{q^k} \leq V_1 \sqrt{\hbar}$$

for all $k \in [0, k^(\hbar, N)]$. Here, $k^*(\hbar, N) = O(\hbar^{-N})$.*

Proof Let $(q, v) \in C$ be positively contained and suppose $|v - X_H(q)|_q < V_0 \hbar$. By Proposition 7, we have

$$|\mu_4(\Psi_\hbar^k(q, v)) - \mu_4(q, v)| \leq \mathcal{M} \hbar,$$

for some N -dependent constant \mathcal{M} and $k \in [0, k^*(\hbar, N)]$. But since $\mu_4(q, v) = \frac{1}{2}|v - X_H(q)|_q^2$ we can apply this inequality to obtain

$$\begin{aligned}
|v^k - X_H(q^k)|_{q^k}^2 &\leq |v^k - X_H(q^k)|_{q^k}^2 - |v - X_H(q)|_q^2 + |v - X_H(q)|_q^2 \\
&\leq 2|\mu_4(\Psi_\hbar^k(q, v)) - \mu_4(q, v)| + V_0^2 \hbar \\
&\leq 2\mathcal{M} \hbar + V_0^2 \hbar.
\end{aligned}$$

Taking a square root gives the desired result. \square

In the above sense, the graph of X_H behaves much like a true invariant set over very large time intervals. Of course, the invariance need not be exact, but may include oscillations around the graph of amplitude $\sqrt{\hbar}$. The amplitude of these oscillations can be reduced by considering manifolds that better approximate the zero level set of μ_{\hbar} , but, as mentioned earlier, we will not pursue this matter further in this article.

To complete the picture of how the symplectic Lorentz map may be used as an integrator for X_H on Q , we will now describe the precise sense in which the map's dynamics approximate the H -flow. We start with a simple estimate that says the q -component of the symplectic Lorentz map approximates the time- \hbar flow of X_H on Q with an $O(\hbar^{5/2})$ error, *provided* the map is applied in an $O(\hbar^{1/2})$ neighborhood of the graph $\{v = X_H(q)\}$.

Proposition 9 *Let (q, v_{\hbar}) be a smooth \hbar -dependent point in TQ with $v_{\hbar} = X_H(q) + O(\hbar^{1/2})$. The mapped point $(\bar{q}, \bar{v}) = \Psi_{\hbar}(q, v_{\hbar})$ satisfies*

$$\begin{aligned}\bar{q} &= q + \hbar X_H(q) + \frac{1}{2}\hbar^2 DX_H(q)[X_H(q)] + O(\hbar^{5/2}), \\ \bar{v} &= X_H(\bar{q}) + O(\hbar^{1/2}).\end{aligned}$$

Proof In the proof of Proposition 5, we already established

$$\begin{aligned}\bar{q} &= x + \frac{1}{2}\hbar X_H(x) + \frac{1}{2}\hbar^2 \Delta(x, v_{\hbar}, \hbar), \\ \bar{v} &= X_H(x) - \exp(-\theta_0 \mathbb{J}_x)[v_{\hbar} - X_H(x)] + O(\hbar),\end{aligned}$$

and

$$\Delta(x, v_{\hbar}, 0) = (1 - \exp(-\theta_0 \mathbb{J}))\mathbb{J}(v_{\hbar} - X_H(x)),$$

where $x = \bar{q}/2 + q/2$. Implicit differentiation of these formulas together with Taylor's theorem with remainder therefore implies

$$\begin{aligned}\bar{q} &= q + \hbar X_H(q) + \frac{1}{2}\hbar^2 DX_H(q)[X_H(q)] + \hbar^2 (1 - \exp(-\theta_0 \mathbb{J}_q))\mathbb{J}_q \\ &\quad (v_{\hbar} - X_H(q)) + O(\hbar^3), \\ \bar{v} &= X_H(q) - \exp(-\theta_0 \mathbb{J}_q)[v_{\hbar} - X_H(q)] + O(\hbar)\end{aligned}$$

The desired result now follows immediately from $v_{\hbar} - X_H(q) = O(\hbar^{1/2})$. \square

Combining this result with our earlier estimate of the normal stability timescale for $\{v = X_H(q)\}$ in Proposition 8 finally allows us to conclude that the q -component of the symplectic Lorentz map provides a persistent approximation of the H -flow over very large time intervals provided initial conditions are chosen close enough to the graph $\{v = X_H(q)\}$.

Corollary 3 (Persistent approximation property) *Let C be a compact set and let $(q, v_{\hbar}) \in C$ be a smooth \hbar -dependent point in C that is positively contained for*

each \hbar . Also assume $v_{\hbar} = X_H(q) + O(\hbar^{1/2})$. For each $N > 0$ there is an integer $k^*(\hbar, N) = O(\hbar^{-N})$ such that

$$\begin{aligned} q^{k+1} &= q^k + \hbar X_H(q^k) + \frac{1}{2} \hbar^2 DX_H(q^k)[X_H(q^k)] + O(\hbar^{5/2}), \\ v^{k+1} &= X_H(q^{k+1}) + O(\hbar^{1/2}), \end{aligned}$$

for each $k \in [0, k^*(\hbar, N)]$. Here, $(q^k, v^k) = \Psi_{\hbar}^k(q, v_{\hbar})$.

Proof Proposition 8 ensures that the iterates (q^k, v^k) remain within $O(\hbar^{1/2})$ of $\{v = X_H(q)\}$ for k in the desired range. Thus, Proposition 9 applies to each iterate individually, which is precisely the desired result. \square

In summary, we have established the following remarkable properties of the symplectic Lorentz map Ψ_{\hbar} .

1. It is symplectic on TQ , when TQ is endowed with the magnetic symplectic form $\Omega_{\hbar}^* = \pi^* \omega + \hbar^2 \Omega$.
2. Its q -component provides an approximation of the time- \hbar flow of X_H with $O(\hbar^{5/2})$ local truncation error when applied to points in TQ within $O(\hbar^{1/2})$ of $\{v = X_H(q)\}$.
3. If an initial condition is chosen to lie within $\hbar^{1/2}$ of $\{v = X_H(q)\}$ then it will remain within $\hbar^{1/2}$ of the same set for a number of iterations that scales like \hbar^{-N} for any N .

5 Examples

5.1 Hidden-Variable Newtonian Gravity

In this section, we will use nearly periodic maps to construct a discrete-time model of Newtonian gravitation where the gravitational constant has a dynamical origin. Let $M = \mathbb{R} \times \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}^d \ni (q, p, \mathbf{Q}, \mathbf{P})$ and set $\Omega_{\gamma} = dq \wedge dp + \sum_{i=1}^d dQ^i \wedge dP_i$. Let $V, W : \mathbb{R}^d \rightarrow \mathbb{R}$ be smooth functions. The Hamiltonian

$$H_{\epsilon}(q, p, \mathbf{Q}, \mathbf{P}) = \frac{1}{2} (p^2 + q^2) + \epsilon \left(\frac{1}{2} |\mathbf{P}|^2 + V(\mathbf{Q}) + q^2 W(\mathbf{Q}) \right) \quad (24)$$

defines a continuous-time nearly periodic Hamiltonian system with equations of motion

$$\dot{p} = -q - \epsilon 2q W(\mathbf{Q}) \quad (25)$$

$$\dot{q} = p \quad (26)$$

$$\dot{\mathbf{P}} = -\epsilon \partial_{\mathbf{Q}} V - \epsilon q^2 \partial_{\mathbf{Q}} W \quad (27)$$

$$\dot{\mathbf{Q}} = \epsilon \mathbf{P}. \quad (28)$$

The angular frequency function is $\omega_0 = 1$, the limiting roto-rate is $R_0 = -q \partial_p + p \partial_q$, and the corresponding $U(1)$ -action is $\Phi_\theta(q, p, \mathbf{Q}, \mathbf{P}) = (\cos \theta q + \sin \theta p, \cos \theta p - \sin \theta q, \mathbf{Q}, \mathbf{P})$. When $\epsilon = 0$, the system's flow is $F_t(q, p, \mathbf{Q}, \mathbf{P}) = \Phi_t(q, p, \mathbf{Q}, \mathbf{P})$. Intuitively, the (q, p) variables correspond to a fast oscillator that couples nonlinearly to a mechanical system parameterized by (\mathbf{Q}, \mathbf{P}) . The averaged Hamiltonian for the coupled system is

$$\frac{1}{2\pi} \int_0^{2\pi} \Phi_\theta^* H_\epsilon d\theta = \mu_0 + \epsilon \left(\frac{1}{2} |\mathbf{P}|^2 + V(\mathbf{Q}) + \mu_0 W(\mathbf{Q}) \right), \quad (29)$$

where $\mu_0 = \frac{1}{2}(p^2 + q^2)$ is the leading-order adiabatic invariant. We therefore expect the slow variables (\mathbf{Q}, \mathbf{P}) to behave like a particle in d -dimensional space subject to the effective potential $V(\mathbf{Q}) + \mu_0 W(\mathbf{Q})$.

We will construct a Hamiltonian non-resonant nearly periodic map that accurately simulates the slow dynamics for this system while “stepping over” the shortest scale $2\pi/\omega_0 \sim 1$. If $h \in \mathbb{R}$ denotes the temporal step size, these requirements translate into symbols as $1 \ll h \ll \epsilon^{-1}$. Upon introducing the parameters $\delta = 1/h$, $\hbar = \epsilon h$, and $\gamma = (\hbar, \delta)$, we may state our requirement equivalently as $|\gamma| \ll 1$. Our construction will now proceed using the method of mixed-variable generating functions.

The exact Type I generating function for this problem can be characterized by Jacobi's solution of the Hamilton–Jacobi equation, which is given by

$$S(q, \mathbf{Q}, \bar{q}, \bar{\mathbf{Q}}) = \int_0^h [p(t)\dot{q}(t) + \mathbf{P}(t)\dot{\mathbf{Q}}(t) - H(q(t), \mathbf{Q}(t), p(t), \mathbf{P}(t))] dt, \quad (30)$$

where $(q(t), \mathbf{Q}(t), p(t), \mathbf{P}(t))$ satisfies Hamilton's equations, and the boundary conditions $q(0) = q$, $\mathbf{Q}(0) = \mathbf{Q}$, $q(h) = \bar{q}$, $\mathbf{Q}(h) = \bar{\mathbf{Q}}$. In the setting of variational integrators (Marsden and West 2001), this is referred to as the exact discrete Lagrangian, and there are also exact discrete Hamiltonians (Leok and Zhang 2011) corresponding to Type II and Type III generating functions. One possible way to construct a computable approximation of the exact Type I generating function is to observe that it can also be expressed as

$$S(q, \mathbf{Q}, \bar{q}, \bar{\mathbf{Q}}) = \text{ext}_{\substack{(q,p,\mathbf{Q},\mathbf{P}) \in C^2([0,h],M) \\ q(0)=q, q(h)=\bar{q}, \\ \mathbf{Q}(0)=\mathbf{Q}, \mathbf{Q}(h)=\bar{\mathbf{Q}}}} \int_0^h [p(t)\dot{q}(t) + \mathbf{P}(t)\dot{\mathbf{Q}}(t) - H(q(t), \mathbf{Q}(t), p(t), \mathbf{P}(t))] dt, \quad (31)$$

Then, one can construct a computable approximation by replacing the infinite-dimensional function space $C^2([0, h], M)$ with a finite-dimensional subspace, and replacing the integral with a numerical quadrature formula, which yields a Galerkin discrete Lagrangian. Under a number of technical assumptions, the resulting variational integrators Γ -converge to the exact flow map (Müller and Ortiz 2004), and a quasi-optimality result (Hall and Leok 2015) implies that the rate of convergence is

related to the best approximation properties of the finite-dimensional function space used to construct the Galerkin discrete Lagrangian. In general, this means that a good integrator can be constructed by choosing a finite-dimensional function space that is rich enough to approximate the exact solutions well, and using a quadrature rule that is accurate for that choice of function space.

This might entail augmenting the function space with the solution of the fast dynamics when the slow variables are frozen, and then using a quadrature rule that is well adapted to highly oscillatory integrals, like Filon quadrature (Iserles and Nørsett 2004). In this case, the problem exhibits a fast–slow structure that lends itself to a hybrid approximation. We exploit the timescale separation to approximate the fast variables of the dynamics $(q(t), p(t))$ by the exact solution of the $\epsilon = 0$ limiting system,

$$\dot{p} = -q, \quad \dot{q} = p, \quad \dot{P} = 0, \quad \dot{Q} = 0.$$

where the slow variables $(Q(t), P(t))$ are frozen, which leads to a sinusoidal solution for (q, p) . Furthermore, because the timestep h is assumed to be large enough that the fast variables perform many revolutions in that time, we anti-alias the fast dynamics by replacing the revolutions by just the fractional part of the revolutions, which we denote by θ_0 , and which is assumed to be some irrational multiple of 2π , so that the invariant distribution remains the same. The component of the action integral associated with the fast variables can be evaluated analytically in this case. As for the slow variables, we adopt an approach that can be used to derive the implicit midpoint rule, which is a symplectic integrator for Hamiltonian systems. This involves approximating the solution space by linear functions, so $Q(t)$ is uniquely determined by the boundary conditions, and approximating the integral by the midpoint rule. The use of mixed quadrature approximations of the action integral was the basis for implicit–explicit variational integrators for fast–slow systems (Stern and Grinspun 2009).

Note that $\omega_0 = 1$, then for the (q, p) dynamics to have a θ_0 rotation in time h , the solution is given by

$$\begin{bmatrix} q(t) \\ p(t) \end{bmatrix} = \begin{bmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{bmatrix} \begin{bmatrix} q \\ p \end{bmatrix},$$

where $\theta_0/h = 1$. Since $q(t) = \sin(t)p + \cos(t)q$, then $\bar{q} = q(h) = \sin(\theta_0)p + \cos(\theta_0)q$, and hence, $p = \frac{\bar{q} - \cos(\theta_0)q}{\sin(\theta_0)}$. Therefore, the (q, p) dynamics, expressed in terms of the boundary data, is given by

$$\begin{bmatrix} q(t) \\ p(t) \end{bmatrix} = \begin{bmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{bmatrix} \begin{bmatrix} q \\ \frac{\bar{q} - \cos(\theta_0)q}{\sin(\theta_0)} \end{bmatrix} = \begin{bmatrix} \cos(t)q + \sin(t)\frac{\bar{q} - \cos(\theta_0)q}{\sin(\theta_0)} \\ -\sin(t)q + \cos(t)\frac{\bar{q} - \cos(\theta_0)q}{\sin(\theta_0)} \end{bmatrix}.$$

For the slow degrees of freedom, we consider a linear interpolant in time, $Q(t) = Q + \frac{\bar{Q} - Q}{h}t$, from which the momentum becomes $P(t) = \frac{1}{\epsilon} \dot{Q}(t) = \frac{1}{\epsilon} \frac{\bar{Q} - Q}{h}$. Collecting

all of these, we have

$$\begin{aligned} q(t) &= \cos(t)q + \sin(t)\frac{\bar{q} - \cos(\theta_0)q}{\sin(\theta_0)}, \quad \mathbf{Q}(t) = \mathbf{Q} + \frac{\bar{\mathbf{Q}} - \mathbf{Q}}{h}t, \\ \dot{q}(t) &= -\sin(t)q + \cos(t)\frac{\bar{q} - \cos(\theta_0)q}{\sin(\theta_0)}, \quad \dot{\mathbf{Q}}(t) = \frac{\bar{\mathbf{Q}} - \mathbf{Q}}{h}, \\ p(t) &= -\sin(t)q + \cos(t)\frac{\bar{q} - \cos(\theta_0)q}{\sin(\theta_0)}, \quad \mathbf{P}(t) = \frac{1}{\epsilon}\frac{\bar{\mathbf{Q}} - \mathbf{Q}}{h}. \end{aligned}$$

With these, we are now ready to approximate the exact Type I generating function,

$$\begin{aligned} S(q, \mathbf{Q}, \bar{q}, \bar{\mathbf{Q}}) &= \int_0^h [p(t)\dot{q}(t) + \mathbf{P}(t)\dot{\mathbf{Q}}(t) - H(q(t), \mathbf{Q}(t), p(t), \mathbf{P}(t))] dt \\ &= \int_0^h \left[p(t)\dot{q}(t) - \frac{1}{2}(p(t)^2 + q(t)^2) \right. \\ &\quad \left. + \mathbf{P}(t)\dot{\mathbf{Q}}(t) - \epsilon \left(\frac{1}{2}|\mathbf{P}(t)|^2 + V(\mathbf{Q}(t)) + q(t)^2 W(\mathbf{Q}(t)) \right) \right] dt, \end{aligned}$$

where we observe that the integral involving the (q, p) terms has the form of an trigonometric integral, which can be evaluated analytically,

$$\begin{aligned} &\int_0^h \left[p(t)\dot{q}(t) - \frac{1}{2}(p^2 + q^2) \right] \\ &= \int_0^h \left[(p^2 \cos^2(t) - 2pq \cos(t) \sin(t) + q^2 \sin^2(t)) - \frac{1}{2}(p^2 + q^2) \right] dt \\ &= \int_0^h \left[\left(p^2 \left(\frac{1 + \cos(2t)}{2} \right) - pq \sin(2t) + q^2 \left(\frac{1 - \cos(2t)}{2} \right) \right) - \frac{1}{2}(p^2 + q^2) \right] dt \\ &= \int_0^h \left[\left(\frac{1}{2}(p^2 - q^2) \cos(2t) - pq \sin(2t) \right) \right] dt \\ &= \frac{1}{4}(p^2 - q^2) \sin(2t) + \frac{1}{2}pq \cos(2t) \Big|_0^{\theta_0} \\ &= \frac{\cos(\theta_0)\frac{1}{2}\bar{q}^2 + \cos(\theta_0)\frac{1}{2}q^2 - q\bar{q}}{\sin(\theta_0)} \end{aligned}$$

where we made use of the trigonometric double angle formulas, $p = \frac{\bar{q} - \cos(\theta_0)q}{\sin(\theta_0)}$, and $h = \theta_0$. It is easy to verify that this generating function generates a θ_0 rotation in the (q, p) variables.

We approximate the integral involving the (\mathbf{Q}, \mathbf{P}) terms with the midpoint rule,

$$\int_0^h \left[\mathbf{P}(t)\dot{\mathbf{Q}}(t) - \epsilon \left(\frac{1}{2}|\mathbf{P}(t)|^2 + V(\mathbf{Q}(t)) + q(t)^2 W(\mathbf{Q}(t)) \right) \right] dt$$

$$\begin{aligned}
&\approx h \left[\frac{1}{\epsilon} \left(\frac{\overline{\mathbf{Q}} - \mathbf{Q}}{h} \right)^2 - \epsilon \left(\frac{1}{2} \frac{1}{\epsilon^2} \left(\frac{\overline{\mathbf{Q}} - \mathbf{Q}}{h} \right)^2 + V \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right) \right. \right. \\
&\quad \left. \left. + q \left(\frac{h}{2} \right)^2 W \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right) \right) \right] \\
&= h \left[\frac{1}{2\epsilon} \left(\frac{\overline{\mathbf{Q}} - \mathbf{Q}}{h} \right)^2 - \epsilon \left(V \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right) + q \left(\frac{h}{2} \right)^2 W \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right) \right) \right].
\end{aligned}$$

By using $\hbar = \epsilon h$, replacing $q \left(\frac{h}{2} \right)$ with $q(0) = q$, and combining it with the first term coming from the fast dynamics, we obtain the following Type I generating function:

$$\begin{aligned}
S_\gamma(q, \mathbf{Q}, \overline{q}, \overline{\mathbf{Q}}) &= \frac{\cos \theta_0 \frac{1}{2} q^2 + \cos \theta_0 \frac{1}{2} \overline{q}^2 - q \overline{q}}{\sin \theta_0} + \frac{1}{2} \frac{|\overline{\mathbf{Q}} - \mathbf{Q}|^2}{\hbar} \\
&\quad - \hbar V \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right) - \hbar q^2 W \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right), \quad (32)
\end{aligned}$$

where θ_0 is some irrational multiple of 2π . The implicit relations

$$\overline{p} = \partial_{\overline{q}} S_\gamma, \quad p = -\partial_q S_\gamma, \quad \overline{\mathbf{P}} = \partial_{\overline{\mathbf{Q}}} S_\gamma, \quad \mathbf{P} = -\partial_{\mathbf{Q}} S_\gamma, \quad (33)$$

define a γ -dependent symplectic map $F_\gamma : (q, p, \mathbf{Q}, \mathbf{P}) \mapsto (\overline{q}, \overline{p}, \overline{\mathbf{Q}}, \overline{\mathbf{P}})$. For small γ , we claim this map accurately captures the averaged dynamics of the slow variables in the system (25)–(28) and preserves the adiabatic invariant μ_0 over very large time intervals. To show this, we first compute the derivatives in (33) to explicitly write the defining equations for F_γ as

$$\begin{aligned}
\overline{p} &= \frac{\cos \theta_0}{\sin \theta_0} \overline{q} - \frac{1}{\sin \theta_0} q, \\
p &= -\frac{\cos \theta_0}{\sin \theta_0} q + \frac{1}{\sin \theta_0} \overline{q} + \hbar 2q W \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right), \\
\overline{\mathbf{P}} &= \frac{\overline{\mathbf{Q}} - \mathbf{Q}}{\hbar} - \frac{1}{2} \hbar V' \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right) - \frac{1}{2} \hbar q^2 W' \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right), \\
\mathbf{P} &= \frac{\overline{\mathbf{Q}} - \mathbf{Q}}{\hbar} + \frac{1}{2} \hbar V' \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right) + \frac{1}{2} \hbar q^2 W' \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right).
\end{aligned}$$

The first pair of equations can be solved explicitly for \overline{p} and \overline{q} , giving

$$\overline{p} = \cos \theta_0 p - \sin \theta_0 q - \cos \theta_0 \hbar 2q W \left(\frac{\mathbf{Q} + \overline{\mathbf{Q}}}{2} \right), \quad (34)$$

$$\bar{q} = \cos \theta_0 q + \sin \theta_0 p - \sin \theta_0 \hbar 2q W \left(\frac{\mathbf{Q} + \bar{\mathbf{Q}}}{2} \right). \quad (35)$$

Adding and subtracting the last \mathbf{P} and $\bar{\mathbf{P}}$ equations then gives

$$\bar{\mathbf{P}} - \mathbf{P} = -\hbar V' \left(\frac{\mathbf{Q} + \bar{\mathbf{Q}}}{2} \right) - \hbar q^2 W' \left(\frac{\mathbf{Q} + \bar{\mathbf{Q}}}{2} \right), \quad (36)$$

$$\bar{\mathbf{Q}} - \mathbf{Q} = \hbar \frac{\mathbf{P} + \bar{\mathbf{P}}}{2}. \quad (37)$$

These formulas show that $F_0 = \Phi_{\theta_0}$, which implies that F_γ comprises a non-resonant, Hamiltonian, nearly periodic map. In particular, this map admits an all-orders adiabatic invariant $\mu = \mu_0 + \hbar \mu_1 + O(\hbar^2)$, where

$$\begin{aligned} \mu_0 &= \frac{1}{2}(q^2 + p^2) \\ \mu_1 &= -\frac{1}{2}W(\mathbf{Q}) \left(2pq + (p-q)(p+q) \cot \theta_0 \right). \end{aligned}$$

Moreover, Eqs. (36) and (37) provide a consistent numerical scheme for the averaged dynamics of the slow variables. To see this, observe that the average of q^2 in (36) after many iterations tends to μ_0 , which implies that, on average, (36) and (37) comprise the implicit midpoint scheme applied to the continuous system's averaged dynamics. Note that the relationship between the physical timestep h and \hbar is $h = \hbar/\epsilon$. Also note that the approximation $q(h/2) \approx q(0)$ used when approximating the action integral is not systematic due to the rapid oscillations in $q(t)$. This was done merely for the sake of obtaining an especially simple time advance. A more systematic approach would adopt Filon-type quadrature for the part of the integrand involving both slowly and rapidly varying terms, but the resulting nearly periodic map would have the same qualitative properties as the one introduced here.

A planar N -body problem in Cartesian (x, y) -coordinates provides a convenient sandbox for testing the novel scheme (34)–(37). Assume two bodies, labeled by the position vectors $\mathbf{Q}_1 = (Q_{1,x}, Q_{1,y})$ and $\mathbf{Q}_2 = (Q_{2,x}, Q_{2,y})$ and the respective momentum vectors $\mathbf{P}_1 = (P_{1,x}, P_{1,y})$ and $\mathbf{P}_2 = (P_{2,x}, P_{2,y})$, to orbit an infinitely massive body at the origin. The potential $V(\mathbf{Q})$ is therefore

$$V(\mathbf{Q}_1, \mathbf{Q}_2) = -\frac{1}{|\mathbf{Q}_1|} - \frac{1}{|\mathbf{Q}_2|}. \quad (38)$$

Also assume the two bodies to interact via the additional central potential

$$W(\mathbf{Q}_1, \mathbf{Q}_2) = -\frac{1}{|\mathbf{Q}_1 - \mathbf{Q}_2|}. \quad (39)$$

The instantaneous value of q^2 therefore indicates the strength of the coupling of the two bodies via the temporal evolution of the ϵ -perturbed (q, p) oscillator.

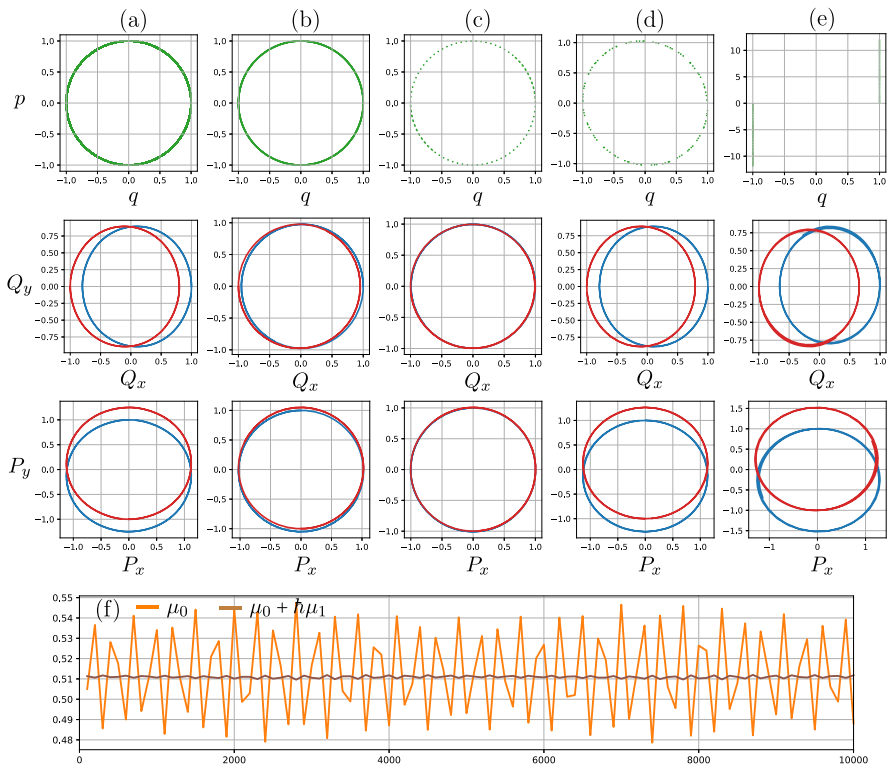


Fig. 1 Numerical solutions of the hidden-variable Newtonian gravity example for $\epsilon = 0.001$ and maximum integration time $T = 10000$. The green trajectories on the top row denote the fast variable pair (q, p) . The blue and red trajectories on the mid row refer to the positions (Q_x, Q_y) of the particles one and two in Cartesian coordinates, and to their respective momentums (P_x, P_y) on the bottom row. The columns (a), (b), and (c) correspond to implicit midpoint scheme with time steps $h = 0.1$, $h = 4.0$, and $h = 100.0$, respectively. The columns (d) and (e) correspond to the fast-slow scheme with a time step of $h = 100.0$ and the angle variable being (d) non-resonant $\theta_0 = 2.0$ and (e) resonant $\theta_0 = \pi$. The large panel (f) at the bottom displays the time trace of the adiabatic invariant, corresponding to the fast-slow trajectory of column (d). The column (a) can be considered as the reference solution which the non-resonant fast-slow scheme reproduces quite well in the column (d)

The behavior of the scheme (34)–(37) is illustrated in Fig. 1 together with the numerical solution from the well-known implicit midpoint scheme which is symplectic for canonical Hamiltonian systems and generally considered a good scheme for stiff problems. For both integrators, we set the system parameter to $\epsilon = 0.001$. In Fig. 1, the columns (a), (b), and (c) correspond to implicit midpoint scheme with time steps $h = 0.1$, $h = 4.0$, and $h = 100.0$, respectively. The columns (d) and (e) correspond to the fast-slow scheme with a time step of $h = 100.0$ and the angle variable being (d) non-resonant $\theta_0 = 2.0$ and (e) resonant $\theta_0 = \pi$. The column (a) can be considered as the reference solution, which the non-resonant fast-slow integrator in column (d) closely matches.

Certain peculiar behavior is evident in the columns (b), (c), and (e). By increasing the time step and “stepping over” the fastest stiff time scale, the implicit midpoint method decouples the fast and slow variables but in an incorrect manner: through the columns (a), (b), and (c), the blue and red orbits gradually transit into co-centric circles, indicating the dependence of the adiabatic invariant μ_0 on the step size h . Explanation for this behavior is rooted in the asymptotic behavior of the scheme, which is made transparent by writing the implicit midpoint scheme in the form

$$\bar{q} + q = -2 \frac{\bar{p} - p}{h} - \epsilon 4 \frac{\bar{q} + q}{2} W \left(\frac{\mathcal{Q} + \bar{\mathcal{Q}}}{2} \right), \quad (40)$$

$$\bar{p} + p = 2 \frac{\bar{q} - q}{h}, \quad (41)$$

$$\bar{P} - P = -h\epsilon V' \left(\frac{\mathcal{Q} + \bar{\mathcal{Q}}}{2} \right) - h\epsilon \frac{(\bar{q} + q)^2}{4} W' \left(\frac{\mathcal{Q} + \bar{\mathcal{Q}}}{2} \right), \quad (42)$$

$$\bar{\mathcal{Q}} - \mathcal{Q} = h\epsilon \frac{P + \bar{P}}{2}. \quad (43)$$

When ϵ is small and the time step h becomes large, the limiting behavior of the fast variables is constant flipping of their signs. Most importantly, the term $\bar{q} + q$ becomes successively smaller with increasing h . Consequently, the force from the coupling potential W effectively drops out from the equation for the slow variables P , resulting in nearly co-centric slow orbits.

Also in column (e), some strange behavior occurs. Via (34) and (35), the resonant value of $\theta_0 = \pi$ results in the following map for the fast variables

$$\bar{p} = -p + h 2q W \left(\frac{\mathcal{Q} + \bar{\mathcal{Q}}}{2} \right), \quad (44)$$

$$\bar{q} = -q, \quad (45)$$

displaying a constant flipping of q , which translates to amplifying flipping in p . This behavior is straightforward to verify for the initial condition $(q, p) = (1.0, 0.0)$. The behavior of the slow variables in the column (e) in Fig. 1 is off from the reference solution and the non-resonant case but, because the dependence of (36) is only on q and not on the midpoint $(\bar{q} + q)/2$, the solution still exhibits some effect from the coupling potential. Specifically, as the q^2 remains constant and does not average to $(q^2 + p^2)/2$, the effect is actually double that of the one in the reference solution, resulting in the slow orbits being further apart from each other than what they should be.

This example serves to illustrate that even the decorated implicit midpoint scheme is not guaranteed to result in correct asymptotic behavior and that care should be taken in trying to “step over” the stiff time scales. On the other hand, the example also illustrates that an integrator with the correct asymptotic behavior may be constructed,

although care is needed in choosing the saturation value for phase angle for the limit of the nearly periodic map.

5.2 Reduced Guiding-Center Motion

We now apply the general theory developed in Sect. 4.2 to motion of a charged particle in a strong magnetic field of the special form $\mathbf{B}(x, y, z) = B(x, y) \mathbf{e}_z$, where (x, y, z) denotes the usual Cartesian coordinates on \mathbb{R}^3 and B is a positive function. Let $q = (x, y) \in Q = \mathbb{R}^2$ and introduce a symplectic form ω on Q using the formula

$$\omega = -\mathbf{d}\alpha = -B(x, y) dx \wedge dy, \quad \alpha = A_x(x, y) dx + A_y(x, y) dy.$$

Here, the components of the 1-form α may be interpreted as the physicist's vector potential for B . Also define the Hamiltonian function $H : Q \rightarrow \mathbb{R}$ according to

$$H(q) = \mu B(x, y),$$

where μ is a positive constant parameter. The corresponding Hamiltonian vector field is given by

$$X_H = \mathcal{R}_{\pi/2} \mu \nabla \ln B,$$

where $\mathcal{R}_{\pi/2}$ is the rotation matrix \mathcal{R}_θ evaluated at $\pi/2$,

$$\mathcal{R}_\theta = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}.$$

Physically, this Hamiltonian vector field describes the motion of a charged particle's guiding center (Northrop 1963) (x, y) . The parameter μ is the magnetic moment, and X_H is also known as the ∇B -drift velocity. We remark that readers familiar with the Hamiltonian formulation of guiding center motion (Littlejohn 1981; Cary and Brizard 2009) may be used to seeing these equations derived from the Lagrangian $L : TQ \rightarrow \mathbb{R}$ given by

$$L(q, \dot{q}) = \alpha_q(\dot{q}) - H(q).$$

We also remark that in this formulation of guiding center dynamics we have used translation invariance along z to eliminate the (constant) velocity along the magnetic field and the corresponding ignorable coordinate z .

In order to construct the symplectic Lorentz map for this system, we begin by observing that the complex structure

$$\mathbb{J} \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix}$$

is compatible with ω since

$$\omega(\dot{q}_1, \mathbb{J}\dot{q}_2) = B(x, y) \dot{q}_1 \cdot \dot{q}_2,$$

where \cdot denotes the usual inner product on \mathbb{R}^2 . We may therefore use the metric $g_q(v, w) = B(x, y)v \cdot w$ to build a new Hamiltonian system on TQ , compatible with the Lorentz-embedding idea from Burby and Hirvijoki (2021),

$$\Omega_\epsilon^* = \pi^*\omega - \epsilon \mathbf{d}(g_q(v, dq)), \quad H_\epsilon^*(q, v) = \frac{1}{2}\epsilon^2 g_q(v, v) + \epsilon \tau H(q),$$

where we have also introduced a constant factor τ for scaling time of the original system. This scaling will help us later to assign the fastest motion in the guiding center system to occur at order one and help in nonlinear solve of the coordinate update map in our numerical example. Essentially, the true time of the original system now evolves at rate that is τ times the rate of the embedded system. The equations of motion for this larger system are given by

$$\begin{aligned} \dot{q} &= \epsilon v, \\ \dot{v} &= -(1 + \epsilon v \cdot \mathcal{R}_{\pi/2} \cdot \nabla \ln B) \mathcal{R}_{\pi/2} v - \left(\tau \mu + \epsilon \frac{1}{2} |v|^2 \right) \nabla \ln B. \end{aligned}$$

Proceeding now with the general construction of the symplectic Lorentz map, we introduce a Type I generating function

$$S(q, \bar{q}) = \int_q^{\bar{q}} \alpha + \Sigma(q/2 + \bar{q}/2, \bar{q} - q),$$

where $\Sigma : TQ \rightarrow \mathbb{R}$ is given by

$$\begin{aligned} \Sigma(\eta, \xi) &= -\hbar \mu B(\eta) + \hbar^2 B(\eta) X_H(\eta) \cdot \xi \\ &\quad - \frac{1}{4} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) B(\eta) (\xi - \hbar X_H(\eta)) \cdot (\xi - \hbar X_H(\eta)). \end{aligned}$$

Note we are using the symbol η instead of x , in contrast to Sect. 4.2, in order to avoid confusion with the standard Cartesian coordinate system. The term involving derivatives of ω , present in the previous section, vanishes identically for $X_H \cdot \nabla B = 0$. The symplectic Lorentz map then provides the equations

$$\begin{aligned} \hbar^2 B(\bar{q}) \bar{v} &= - \int_0^1 \lambda B(q + \lambda \xi) d\lambda \mathcal{R}_{\pi/2} \xi + \frac{1}{2} \partial_\eta \Sigma(\eta, \xi) + \partial_\xi \Sigma(\eta, \xi), \\ \hbar^2 B(q) v &= \int_0^1 (1 - \lambda) B(q + \lambda \xi) d\lambda \mathcal{R}_{\pi/2} \xi - \frac{1}{2} \partial_\eta \Sigma(\eta, \xi) + \partial_\xi \Sigma(\eta, \xi), \end{aligned}$$

where the derivatives are

$$\begin{aligned}\partial_{\eta} \Sigma(\eta, \xi) &= -\hbar\mu \nabla B(\eta) + \hbar^2 \nabla B(\eta) X_H(\eta) \cdot \xi + \hbar^2 B(\eta) \nabla X_H(\eta) \cdot \xi \\ &\quad - \frac{1}{4} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) \nabla B(\eta) (\xi - \hbar X_H(\eta)) \cdot (\xi - \hbar X_H(\eta)) \\ &\quad + \frac{1}{2} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) B(\eta) \hbar \nabla X_H(\eta) \cdot (\xi - \hbar X_H(\eta)), \\ \partial_{\xi} \Sigma(\eta, \xi) &= \hbar^2 B(\eta) X_H(\eta) - \frac{1}{2} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) B(\eta) (\xi - \hbar X_H(\eta)),\end{aligned}$$

and everything is understood to be evaluated at $(\eta, \xi) = ((\bar{q} + q)/2, \bar{q} - q)$.

Next, we rearrange the implicit equation for \bar{q} into

$$\begin{aligned}&\left[\frac{1}{2} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) B(\eta) 1 - \int_0^1 (1 - \lambda) B(q + \lambda \xi) d\lambda \mathcal{R}_{\pi/2} \right] \xi \\ &= \left[\frac{1}{2} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) B(\eta) 1 - \frac{1}{2} B(\eta) \mathcal{R}_{\pi/2} \right] \hbar X_H(\eta) \\ &\quad + \hbar^2 B(\eta) X_H(\eta) - \hbar^2 B(q) v - \frac{1}{2} \hbar^2 \nabla B(\eta) X_H(\eta) \cdot \xi - \frac{1}{2} \hbar^2 B(\eta) \nabla X_H(\eta) \cdot \xi \\ &\quad + \frac{1}{8} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) \nabla B(\eta) (\xi - \hbar X_H(\eta)) \cdot (\xi - \hbar X_H(\eta)) \\ &\quad - \frac{1}{4} \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) B(\eta) \hbar \nabla X_H(\eta) \cdot (\xi - \hbar X_H(\eta)),\end{aligned}$$

which can be iterated for η and ξ . After that, one solves for \bar{v} by evaluating, for example, the expression

$$\begin{aligned}\hbar^2 B(\bar{q}) \bar{v} + \hbar^2 B(q) v &= - \int_0^1 \lambda B(q + \lambda \xi) d\lambda \mathcal{R}_{\pi/2} \xi + \int_0^1 (1 - \lambda) B(q + \lambda \xi) d\lambda \mathcal{R}_{\pi/2} \xi \\ &\quad + 2\hbar^2 B(\eta) X_H(\eta) - \left(\frac{\sin \theta_0}{1 - \cos \theta_0} \right) B(\eta) (\xi - \hbar X_H(\eta)).\end{aligned}$$

Next, we perform some numerical tests. First, we choose a magnetic field

$$B = B_0(1 + \alpha|q|^2),$$

where α introduces a small perturbation to the otherwise constant magnetic field. For the original system $\dot{q} = X_H(q)$, this field results in circular orbits for q . We then investigate the solutions of the symplectic Lorentz map and compare them with the classic RK4 integrator and the implicit midpoint applied to the original system. For the scaling of time, we choose $\tau = \alpha^{-1}$. Choosing an initial point $q = (1, 1)$, parameters $B_0 = 1$, $\mu = 1.0$, $\alpha = 0.001$, and initializing the Lorentz map with $v = X_H(q)$, we run the simulation for 60'000 steps of size $\hbar = 0.1$. This is enough to demonstrate the

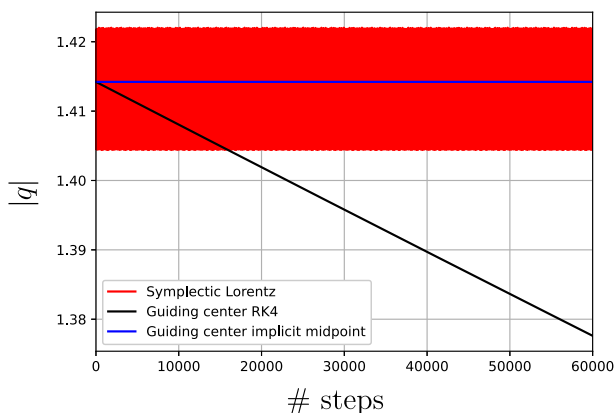


Fig. 2 Comparison of the guiding-center RK4 integrator, implicit midpoint, and the symplectic Lorentz map in the simple magnetic field case. The orbit radius $|q|$ of the RK4 integrator deteriorates clearly while the symplectic Lorentz map and the implicit midpoint manage to retain the radius within stable limits

Table 1 Cost performance of different integrators

| | RK4 | Implicit midpoint | Symplectic Lorentz |
|-------------------------|-----|-------------------|--------------------|
| Average # of iterations | 1 | 16 | 22 |
| Average execution time | 1.4 | 21 | 128 |

deterioration of the RK4 method while the symplectic Lorentz map and the implicit midpoint preserve the orbit in place, as seen in Fig. 2. The average number of iterations for solving the discrete system of equations and the average total execution times for the different algorithms are recorded in Table 1. Solving the nonlinear equations to machine precision results on average 16 iterations for the implicit midpoint and 22 iterations for the symplectic Lorentz map during every time step. The execution time of the Lorentz map is approximately six times that of the implicit midpoint method, credited to the larger number of iterations required and the need for additional quantities to be evaluated, such as the line integrals present in the generating function. This limited comparison with other methods should not be construed as the last word on the subject. The important takeaways include (a) the number of implicit iterations needed for one step of the symplectic Lorentz map is comparable to the number of iterations required for implicit midpoint applied to the original problem, even though the number of function evaluations is higher for symplectic Lorentz, (b) the symplectic Lorentz map achieves similar long-time solution quality as a popular scheme for integrating non-dissipative systems, and (c) the symplectic Lorentz map has provable structure-preserving properties, while implicit midpoint does not in this case. (Implicit midpoint is known to be symplectic for canonical Hamiltonian systems, but not in general for non-canonical systems like the one considered here.)

Next, we consider the magnetic field

$$B(x, y) = 2 + y^2 - x^2 + \frac{1}{4}x^4,$$

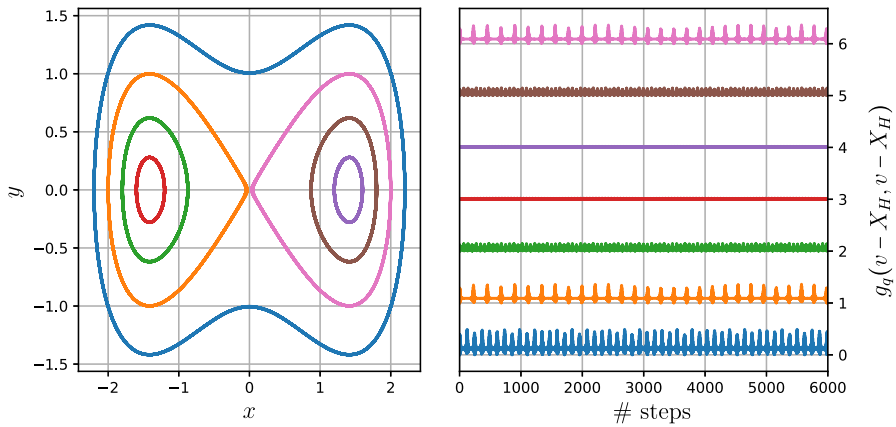


Fig. 3 Phase-space orbits (left) and the adiabatic invariant (right). For the “figure-eight” magnetic field. The values of the adiabatic invariant have been shifted by the integers $\{0, \dots, 6\}$ for illustrative purposes. A lesser number of steps (6000) have been chosen to illustrate the non-trivial beating structure of the adiabatic invariant

whose level sets have a “figure-eight” structure. By energy conservation, the guiding-center orbits should reflect this pattern. Choosing a time step of $\hbar = 0.05$ and $\tau = 1.0$, we run the symplectic Lorentz map for 6'000 steps and illustrate both the orbits and the evolution of the postulated adiabatic invariant $g_q(v - X_H, v - X_H)$ in Fig. 3. The orbits appear stable and well-confined to their respective phase-space domains, and the adiabatic invariant remains within bounds while oscillating with a non-trivial beating structure.

For the same magnetic field, we performed a pair of tests that probe the robustness of the discrete-time adiabatic invariant μ . We introduce an empirical estimate of the breakdown time for μ conservation and compute how that estimate varies with the parameters θ_0 and \hbar . Our estimate is based on the observation that μ typically oscillates about a time-varying mean value $\bar{\mu}$ with an approximately constant oscillation amplitude $\tilde{\mu}$. We estimate that breakdown has occurred after n iterations when $|\bar{\mu}(n\hbar) - \bar{\mu}(0)| > \tilde{\mu}$. We then define the breakdown time estimate to be $T_{\text{breakdown}} = n\hbar$. Results from our sensitivity studies are displayed in Fig. 4. While the general theory predicts that the breakdown time should scale as fast as \hbar^{-N} for any nonnegative integer N , the observable asymptote in $T_{\text{breakdown}}(\hbar)$ appears well-approximated by $\hbar^{-3.5}$. We presently lack understanding of the origin of the scaling exponent -3.5 . The theory also predicts that adiabatic invariance should be less robust when $\theta_0/2\pi$ is rational. This prediction is consistent with the plot of $T_{\text{breakdown}}(\theta_0)$, which shows intermittent depressions in the breakdown time superposed on a strong upward trend as θ_0 approaches π . We hypothesize that these depressions occur at small denominator rational values of $\theta_0/2\pi$ that produce nonlinear self-resonance in the integrator. As with the scaling exponent, we presently lack detailed understanding for the dramatic increase in observed breakdown time as θ_0 approaches π .

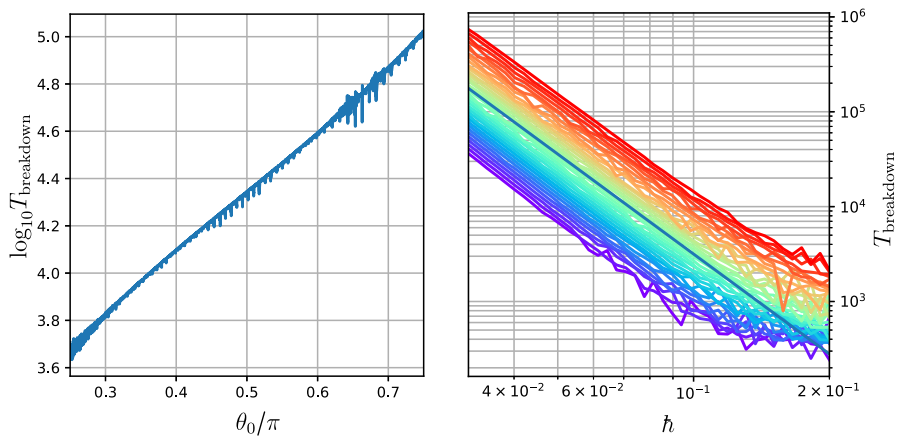


Fig. 4 Left panel: Breakdown time for the adiabatic invariant versus θ_0 . Timestep is fixed at $h = 0.05565$. Initial condition is $x = 2.0$, $y = 0.0$. Right panel: Breakdown time for the adiabatic invariant versus h . Colorscale indicates value of θ_0 , ranging from $\theta_0 = \pi/4$ (purple) to $\theta_0 = 3\pi/4$ (red). Initial condition is $x = 2.0$, $y = 0.0$. Central dark green line is $h^{-3.5}$, for reference. Theory predicts that the breakdown time should scale like h^{-N} for any positive N when h is small enough. While superpolynomial scaling of the breakdown time as a function of h is not apparent in these computations, it cannot be ruled out given the limited range of h values considered. Computing the breakdown time for appreciably smaller values of h rapidly becomes prohibitively expensive because the adiabatic invariant is so well conserved

6 Discussion

In this article, we have introduced and developed the theoretical foundations of nearly periodic maps. These maps provide a discrete-time analog of Kruskal (1962) continuous-time nearly periodic systems. The limiting dynamics of both nearly periodic systems and nearly periodic maps translate points along the orbits of a principal circle bundle. In the continuous-time case, each limiting trajectory ergodically samples an orbit. In discrete time, non-resonance appears as an additional requirement for ergodic sampling. As a first major application of nearly periodic maps, we used them to construct a class of geometric integrators for Hamiltonian systems on arbitrary exact symplectic manifolds.

Kruskal's principal interest in continuous-time nearly periodic systems came from their relationship to the theory of adiabatic invariants. In the paper (Kruskal 1962), Kruskal showed that nearly periodic systems necessarily admit approximate $U(1)$ -symmetries. He then went on to deduce that this approximate symmetry implies the existence of an adiabatic invariant when the underlying nearly periodic system happens to be Hamiltonian. The theory of nearly periodic maps is satisfying in this respect since it establishes the existence of a discrete-time adiabatic invariant for nearly periodic maps with an appropriate Hamiltonian structure. Moreover, the arguments used in the existence proof parallel those originally used by Kruskal. (See Thm. 4.)

It is useful to place the integrators developed in this article in the context of previous attempts at geometric integration of non-canonical Hamiltonian systems. Based on the observation (Arnold 1989) that Hamiltonian systems on exact symplectic manifolds admit degenerate “phase space Lagrangians” (Cary and Littlejohn 1983), Qin and Guan

(2008) proposed direct application of the theory of variational integration (Marsden and West 2001) to phase space Lagrangians for non-canonical systems. While initial results looked promising, further investigations by Leland Ellison (2016); Ellison et al. (2017) revealed that the most intuitive variational discretizations of phase space Lagrangians typically suffer from unphysical instabilities known as “parasitic modes” (Hairer et al. 2006). As noticed first in Rowley and Marsden (2002), the origin of these parasitic modes is related to a mismatch between the differing levels of degeneracy in the phase space Lagrangian and its discretization. Our integrators may be understood as modifications of those studied by Qin and Ellison that stabilize the parasitic modes over very large time intervals by way of a discrete-time adiabatic invariant. This “adiabatic stabilization” mechanism is conceptually interesting since it suppresses numerical instabilities without resorting to the addition of artificial dissipation. Also of note, adiabatic stabilization differs from the stabilization mechanism proposed by Ellison in Ellison et al. (2017), wherein the phase space Lagrangian is discretized so that it has the same level of degeneracy as its continuous-time counterpart. While Ellison’s “properly degenerate” discretizations apply to a very limited class of non-canonical Hamiltonian systems, (see Ellison et al. 2017 for the precise limitations) the adiabatic stabilization method discussed here applies to any Hamiltonian system on an exact symplectic manifold.

In the preprint (Kraus 2017), Kraus has developed an alternative approach to structure-preserving integration of non-canonical Hamiltonian systems based on projection methods. In contrast to our approach, this technique is designed to produce integrators that preserve the original system’s symplectic form, rather than a symplectic form on a larger space. However, there is no geometric picture for why Kraus’ method ought to have this property. In fact, Kraus finds that geometrically reasonable variants of his method are not symplectic. The structure-preserving properties of our method are easier to understand in this respect, since they follow from the standard theory of mixed-variable generating functions for symplectic maps. Both techniques warrant further investigation.

As a final remark concerning relationships between the theory developed here and previous work, it is worthwhile highlighting the technique introduced by Tao in Tao (2016) for constructing explicit symplectic integrators for non-separable Hamiltonians. The latter technique applies to canonical Hamiltonian systems with general Hamiltonian $H(q, p)$. It proceeds by constructing a canonical Hamiltonian system in a space with double the dimension of the original (q, p) space, and then applying splitting methods to the larger system. Much like the symplectic Lorentz system introduced in Burby and Hirvijoki (2021), and exploited in Sect. 4.2, Tao’s larger system contains a copy of the original system as a normally elliptic invariant manifold. This suggests that Tao’s construction might be interpreted as an application of nearly periodic maps. It is a curious fact, however, that Tao’s error analysis suggests the oscillation frequency around the invariant manifold cannot be made to be arbitrarily large. This indicates nearly periodic map theory is not an appropriate tool for understanding Tao’s results. It would be interesting to investigate whether or not nearly periodic map theory can be used to sharpen Tao’s estimates.

More work is required to develop nearly periodic map machinery, in both theory and practice. The following is a list of just a few of the open theoretical questions in this area.

1. Non-resonant nearly periodic maps and nearly periodic systems admit formal $U(1)$ -symmetries, and therefore formal reductions to the space of $U(1)$ -orbits. Given an arbitrary continuous-time nearly periodic system, are there systematic strategies for constructing nearly periodic maps whose $U(1)$ -reduction approximates the flow of the nearly periodic system's $U(1)$ -reduction? (We provide a simple example where this can be done in Sect. 5.1.) Such maps would provide a good approximation of the original system's dynamics "on average."
2. For a Hamiltonian system on an exact symplectic manifold M , the geometric integrators constructed in this article comprise symplectic mappings on TM that admit approximate invariant manifolds diffeomorphic to M . In light of this diffeomorphism, is there some sense in which our integrators possess an adiabatically invariant symplectic form on M ? (Note that this does not obviously follow from the symplectic property on TM .)
3. A commonly touted benefit of symplectic integration is the long-time approximate preservation of energy. Proofs of this result rely on backward error analysis. Can similar techniques be used to prove that our geometric integrators approximately preserve the original Hamiltonian system's energy, at least over large time intervals? Our initial numerical experiments suggest such a result is satisfied for as long as the discrete-time adiabatic invariant is well-conserved.
4. Our geometric integrators enjoy local $O(\hbar^{5/2})$ accuracy. Are there extensions of these integrators with arbitrarily high-order accuracy?

Acknowledgements The work of JWB was supported by the Los Alamos National Laboratory LDRD program under Project No. 20180756PRD4. It was also supported by a Data-Intensive Scientific Machine Learning grant awarded by the DOE SC program in Advanced Scientific Computing Research (ASCR). The work of EH was supported by the Academy of Finland (Grant No. 315278). Any subjective views or opinions expressed herein do not necessarily represent the views of the Academy of Finland or Aalto University. The work of ML was supported by NSF under grants DMS-1345013, DMS-1813635, by AFOSR under grant FA9550-18-1-0288, and by the DoD under grant HQ00342010023 (Newton Award for Transformative Ideas during the COVID-19 Pandemic).

Data Availability The datasets generated during and/or analyzed during the current study are available from the corresponding author upon reasonable request.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

- Abraham, R., Marsden, J.E.: Foundations of Mechanics. AMS Chelsea publishing. American Mathematical Soc. (2008)
- Arnold, V.I.: Mathematical Methods of Classical Mechanics. Springer (1989)
- Burby, J.W., Hirvijoki, H.: Normal stability of slow manifolds in nearly-periodic Hamiltonian systems. *J. Math. Phys.* **62**, 093506 (2021)
- Burby, J.W., Klotz, T.J.: Slow manifold reduction for plasma science. *Commun. Nonlin. Sci. Numer. Simul.* **89**, 105289 (2020)
- Burby, J.W., Squire, J.: General formulas for adiabatic invariants in nearly periodic hamiltonian systems. *J. Plasma Phys.* **86**, 835860601 (2020)
- Cary, J.R., Brizard, A.J.: Hamiltonian theory of guiding-center motion. *Rev. Mod. Phys.* **81**, 693–738 (2009)
- Cary, J.R., Littlejohn, R.G.: Noncanonical Hamiltonian mechanics and its application to magnetic field line flow. *Ann. Phys.* **151**, 1 (1983)
- Ellison, C.L., Finn, J.M., Burby, J.W., Kraus, M., Qin, H., Tang, W.M.: Degenerate variational integrators for magnetic field line flow and guiding center trajectories. *Phys. Plasmas* **25**, 052502 (2017)
- Hairer, E., Lubich, C., Wanner, G.: Geometric Numerical Integration. Springer (2006)
- Hairer, E., Lubich, C.: Long-time analysis of a variational integrator for charged particle dynamics in a strong magnetic field. *Num. Math.* **144**, 699–728 (2020)
- Hall, J., Leok, M.: Spectral variational integrators. *Numer. Math.* **130**(4), 681–740 (2015)
- Iserles, A., Nørsett, S.P.: On quadrature methods for highly oscillatory integrals and their implementation. *BIT Numer. Math.* **44**(4), 755–772 (2004)
- Kraus, M.: Projected variational integrators for degenerate Lagrangian systems (2017)
- Kruskal, M.: Asymptotic theory of Hamiltonian and other systems with all solutions nearly periodic. *J. Math. Phys.* **3**, 806 (1962)
- Leland Ellison, C.: Development of Multistep and Degenerate Variational Integrators for Applications in Plasma Physics. Doctoral Thesis, Princeton University (2016)
- Leok, M., Zhang, J.: Discrete Hamiltonian variational integrators. *IMA J. Numer. Anal.* **31**(4), 1497–1532 (2011)
- Littlejohn, R.G.: A guiding center Hamiltonian: a new approach. *J. Math. Phys.* **20**, 2445 (1979)
- Littlejohn, R.G.: Hamiltonian formulation of guiding center motion. *Phys. Fluids* **24**, 1730 (1981)
- Littlejohn, R.G.: Hamiltonian formulation of guiding center motion. *Phys. Fluids* **24**(9), 1730–1749 (1981)
- Littlejohn, R.G.: Variational principles of guiding center motion. *J. Plasma Phys.* **29**, 111 (1983)
- Lochak, P.: Hamiltonian perturbation theory: periodic orbits, resonances and intermittency. *Nonlinearity* **6**, 885–904 (1993)
- Marsden, J.E., Ratiu, T.S.: Introduction to Mechanics and Symmetry. Texts in Applied Mathematics, vol. 17. Springer, New York (1999)
- Marsden, J.E., West, M.: Discrete mechanics and variational integrators. *Acta Numer.* **10**, 317–514 (2001)
- Müller, S., Ortiz, M.: On the γ -convergence of discrete dynamics and variational integrators. *J. Nonlinear Sci.* **14**(3), 279–296 (2004)
- Northrop, T.G.: The Adiabatic Motion of Charged Particles. Interscience Publishers, Interscience tracts on physics and astronomy (1963)
- Qin, H., Guan, X.: Variational symplectic integrator for long-time simulations of the guiding-center motion of charged particles in general magnetic fields. *Phys. Rev. Lett.* **100**(3), 035006 (2008)
- Ricketson, L.F., Chacón, L.: An energy-conserving and asymptotic-preserving charged-particle orbit implicit time integrator for arbitrary electromagnetic fields. *J. Comput. Phys.* **418**, 109639 (2020)
- Rowley, C.W., Marsden, J.E.: Variational integrators for degenerate Lagrangians, with application to point vortices. 41st IEEE Conference on Decision and Control, vol 40, 1521 (2002)
- Stern, A., Grinspun, E.: Implicit-explicit variational integration of highly oscillatory problems. *Multiscale Model. Simul.* **7**(4), 1779–1794 (2009)
- Tao, M.: Explicit symplectic approximation of nonseparable Hamiltonians: algorithm and long-time performance. *Phys. Rev. E* **94**, 043303 (2016)
- Xiao, J., Qin, H.: Slow manifolds of classical pauli particle enable structure-preserving geometric algorithms for guiding center dynamics. *Comput. Phys. Commun.* **265**, 107981 (2021)