Geometric integration of Hamiltonian systems on exact symplectic manifolds*

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*LA-UR-21-31371, **arXiv:2112.08527**

The phase space for a non-dissipative systems has a frozen-in flux

Frozen-in Flux

$$\boxed{\mathcal{L}_V \omega = 0} \iff \boxed{\delta \int_{t_1}^{t_2} L \, dt = 0}$$

Hamilton's Principle

N.B.: Steady-state MHD frozen-in law is equivalent to
$\mathcal{L}_{\boldsymbol{u}}(\boldsymbol{B} \cdot d\boldsymbol{S}) = (\nabla \times (\boldsymbol{B} \times \boldsymbol{u})) \cdot d\boldsymbol{S} = 0.$

Flux tensor (aka presymplectic form) defines geometry of phase space

Euclidean Geometry	PhaseSpace Geometry
• Metric tensor : g_{ij}	• Flux tensor : ω_{ij} (pre symplectic form)
• Symmetry : $g_{ij} = g_{ji}$ (measures lengths)	• Skew-Symmetry : $\omega_{ij} = -\omega_{ji}$ (measures areas)
• No Curvature : $R^{\rho}{}_{\sigma\mu\nu} = 0$	• No monopoles : $\partial_i \omega_{jk} + \partial_j \omega_{ki} + \partial_k \omega_{ij} = 0$

(pre)Symplectic integrators approximate flow while freezing flux exactly

Definition: symplectic integrator

A **symplectic integrator** for a Hamiltonian ODE $\dot{z}^i = X^i(z)$ is an approximation of the time-advance map

$$F^i(z_0, h) \approx z^i(z_0, h),$$

that satisfies the frozen-flux condition exactly

$$\frac{\partial F^{k_1}}{\partial z_0^i}\, \omega_{k_1\, k_2}(F(z_0, h))\, \frac{\partial F^{k_2}}{\partial z_0^j} = \omega_{ij}(z_0).$$

Symplectic integrators can readily be found when ω_{ij} is canonical

The canonical case

$$\omega_{ij} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

symplectic integrators of any order readily constructed using various techniques

But the non-canonical case is poorly undestood

The noncanonical case

$$\omega_{ij}(z) = \text{anything antisymmetric that satisfies:}$$
$$\partial_i \omega_{jk}(z) + \partial_j \omega_{ki}(z) + \partial_k \omega_{ij}(z) = 0$$

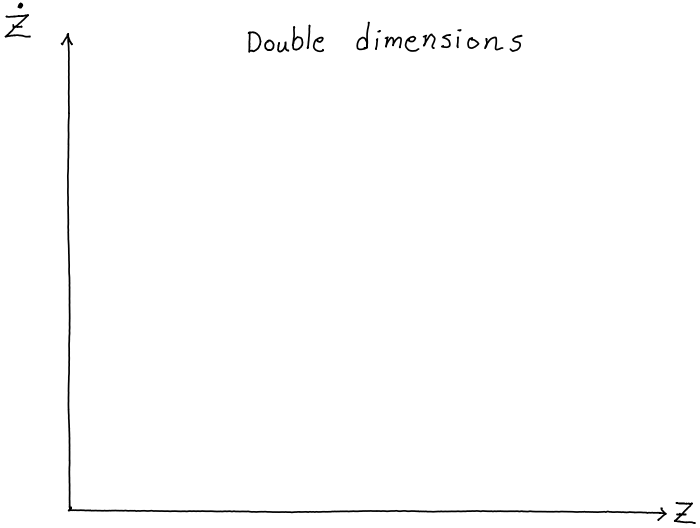
- most interesting systems fall into noncanonical case
- One proposed method* for (almost) general case, but proof of symplectic property difficult to understand

* M. Kraus, "Projected variational integrators for degenerate Lagrangian systems," (arXiv:1708.07356, 2017)

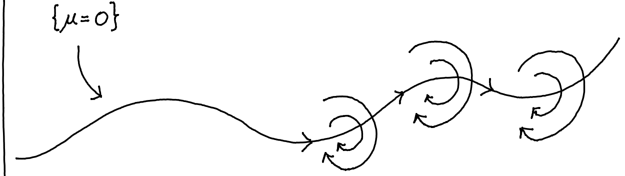
We have developed a new approach to structure-preserving integration of non-dissipative systems that assumes **only**:

1. **Non-degeneracy**: ω_{ij} invertible
2. **Exactness**: $\omega_{ij} = \partial_j \theta_i - \partial_i \theta_j$

Double dimensions



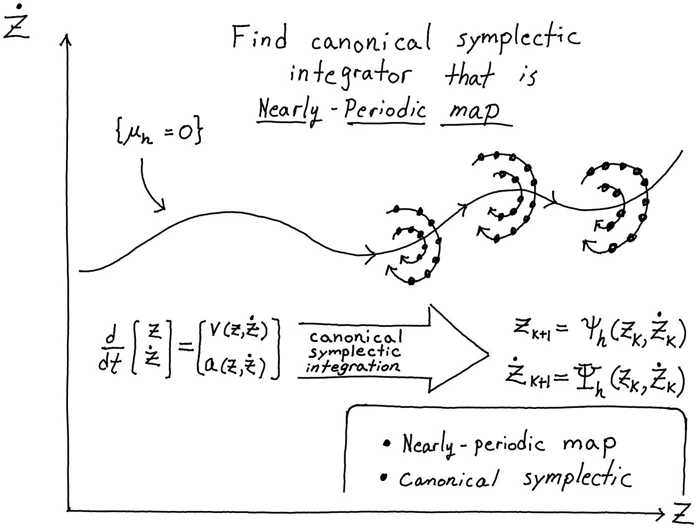
Embed original dynamics
as approximate invariant manifold



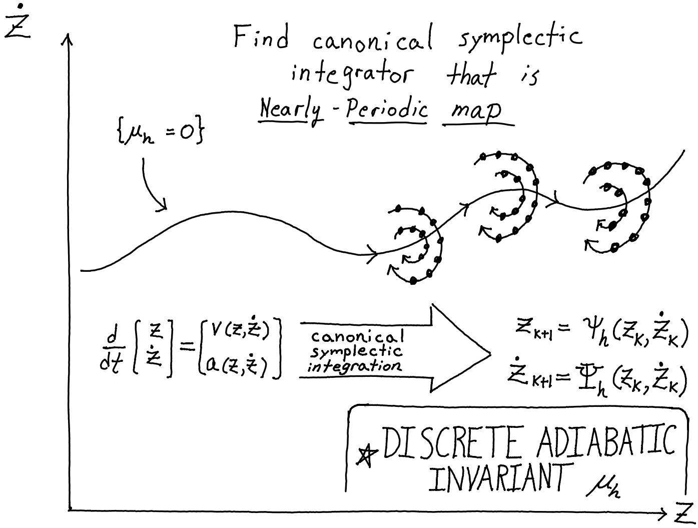
$\dot{z}$ ↑ → z

$$\frac{d}{dt}\begin{bmatrix} z \\ \dot{z} \end{bmatrix} = \begin{bmatrix} v(z,\dot{z}) \\ a(z,\dot{z}) \end{bmatrix}$$

- Nearly-periodic
- Canonical Hamiltonian
- $\mu = 0$ dynamics recovers $\dot{z} = X(z)$



Find canonical symplectic integrator that is Nearly-Periodic map
$\{\mu_h = 0\}$
$\dot{z}$
z
$\frac{d}{dt}\begin{bmatrix} z \\ \dot{z} \end{bmatrix} = \begin{bmatrix} v(z,\dot{z}) \\ a(z,\dot{z}) \end{bmatrix}$
canonical symplectic integration
$z_{k+1} = \Psi_h(z_k, \dot{z}_k)$
$\dot{z}_{k+1} = \Phi_h(z_k, \dot{z}_k)$
• Nearly-periodic map
• Canonical symplectic



Find canonical symplectic integrator that is
Nearly-Periodic map
$\{\mu_h = 0\}$
$\dot{z}$
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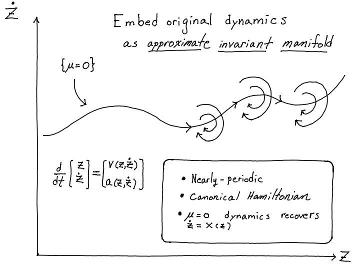
canonical symplectic integration
$z_{k+1} = \Psi_h(z_k, \dot{z}_k)$
$\dot{z}_{k+1} = \Phi_h(z_k, \dot{z}_k)$
☆ DISCRETE ADIABATIC INVARIANT μ_h

Part I: Symplectic Lorentz embedding



Hamilton's equation

$$V^i \omega_{ij} = \partial_j H$$

Hamilton's equation

$$\underbrace{V^i}_{\text{Generator of dynamics}} \qquad \omega_{ij} = \partial_j H$$

Hamilton's equation has an electromagnetic interpretation

Hamilton's equation

$$V^i \underbrace{\omega_{ij}}_{\text{flux tensor}} = \partial_j H$$

Hamilton's equation

$$V^i \omega_{ij} = \underbrace{\partial_j H}_{\text{Hamiltonian}}$$

Hamilton's equation

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electrostatic field

Hamilton's equation

$$V^i \underbrace{\omega_{ij}}_{\text{flux tensor}} = \partial_j H$$

magnetostatic field

Electromagnetic analogue

$$\boldsymbol{v} \times \boldsymbol{B} = -\boldsymbol{E}$$

Electromagnetic analogue

$$\frac{m}{q}\dot{\boldsymbol{v}} = \boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}$$

Zero-mass limit of Lorentz force

This motivates the study of charged particle motion in these "electromagnetic fields"

Lorentz force	"Symplectic" Lorentz force
$\boldsymbol{E}$	$\mathbf{d}H$
$\boldsymbol{B}$	ω
$\frac{1}{2}m\lvert\boldsymbol{v}\rvert^2$	???

But what to do about the mass? (remember $E = mc^2$)

We define mass (kinetic energy) by introducing "compatible almost complex structure"

Def. (almost complex structure)

An **almost complex structure** is a tensor field $\mathbb{J}^i_j$ such that

$$\mathbb{J}^i_k \mathbb{J}^k_j = -\delta^i_j.$$

i.e. $\mathbb{J}$ is a square root of -1.

We define mass (kinetic energy) by introducing "compatible almost complex structure"

Def. (compatible almost complex structure)

Given a flux tensor ω_{ij}, a **compatible almost complex structure** is an almost complex structure $\mathbb{J}^i_j$ such that

$$g_{ij} = \omega_{ik}\mathbb{J}^k_j$$

is symmetric positive definite. i.e. g_{ij} must be a metric tensor.

We define mass (kinetic energy) by introducing "compatible almost complex structure"

Thm. (existence of compatible almost complex structures)

If ω_{ij} is a non-degenerate flux tensor there exists a (non-unique) compatible almost complex structure.

We define mass (kinetic energy) by introducing "compatible almost complex structure"

Lorentz force	"Symplectic" Lorentz force
$\boldsymbol{E}$	$\mathbf{d}H$
$\boldsymbol{B}$	ω
$\frac{1}{2}m\lvert\boldsymbol{v}\rvert^2$	$\frac{1}{2}\epsilon\, g(V, V) \equiv \frac{1}{2}\epsilon\, \omega(V, \mathbb{J}V)$

The symplectic Lorentz system parallels the usual Lorentz force law

Original Hamiltonian system

$$\frac{dZ}{dt} = V(Z), \quad V \cdot \omega = \mathbf{d}H$$

The symplectic Lorentz system parallels the usual Lorentz force law

Symplectic Lorentz system

$$\frac{dZ}{dt} = V, \quad \epsilon \frac{DV}{dt} = \mathbb{J}V - \nabla H$$

properties of symplectic Lorentz system

- Hamiltonian on (Z, V)-space.
  - Flux tensor: $\Omega = \omega + \epsilon\,\Omega_0$
  - Hamiltonian: $\mathcal{H} = H(Z) + \frac{1}{2}\,\epsilon\,g(V, V)$

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- Hamiltonian on (Z, V)-space.
  - Flux tensor: $\Omega = \omega + \epsilon\,\Omega_0$
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- As $\epsilon \to 0$ dynamics becomes periodic

In terms of microscopic time $\tau = t/\epsilon$:

$$\frac{dZ}{d\tau} = \epsilon\, V, \quad \frac{DV}{d\tau} = \mathbb{J}V - \nabla H$$

$$\to \frac{dZ}{d\tau} = 0, \quad \frac{dV}{d\tau} = \mathbb{J}V - \nabla H$$

$$\Rightarrow Z(\tau) = Z(0), \quad V(\tau) = -\mathbb{J}\nabla H + \exp(\tau\,\mathbb{J})[V(0) + \mathbb{J}\nabla H]$$

$\Rightarrow$ **Periodic because $\mathbb{J}^2 = -1$!**

properties of symplectic Lorentz system

- Hamiltonian on (Z, V)-space.
  - Flux tensor: $\Omega = \omega + \epsilon\,\Omega_0$
  - Hamiltonian:$\mathcal{H} = H(Z) + \frac{1}{2}\,\epsilon\, g(V, V)$
- As $\epsilon \to 0$ dynamics becomes periodic
- Has an **adiabatic invariant**:
  - $\mu(Z, V) = \frac{1}{2}\, g(V + \mathbb{J}\nabla H, V + \mathbb{J}\nabla H)$

Thm. (adiabatic invariance)

For each non-negative $k \in \mathbb{Z}$

$$|\mu(t) - \mu(0)| = O(\epsilon), \quad t \in [0, C_k/\epsilon^k]$$

JWB, E. Hirvijoki, *J. Math. Phys.* **62**: 093506 (2021)

$\mu = 0$ dynamics approximates original system

Corollary:

If $\mu (= \frac{1}{2} g(V + \mathbb{J}\nabla H, V + \mathbb{J}\nabla H)) = 0$ then $V = -\mathbb{J}\nabla H$.
In particular, if $\mu(0) = 0$ then for each k

$$\frac{dZ}{dt} = -\mathbb{J}\nabla H + O(\epsilon^{1/2}), \quad t \in [0, C_k/\epsilon^k]$$

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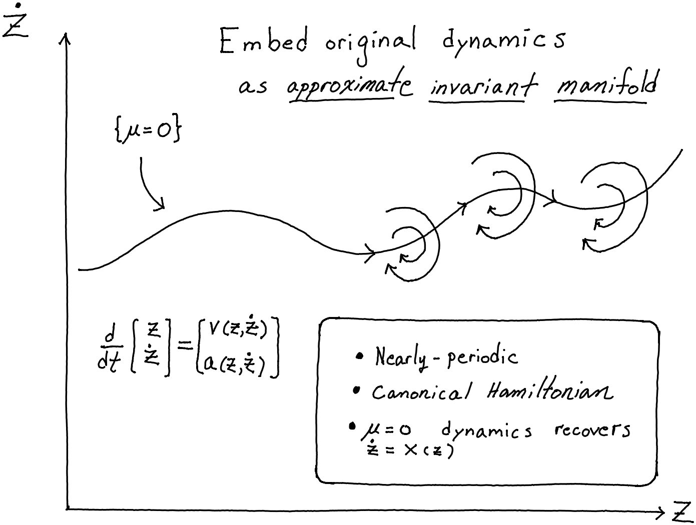
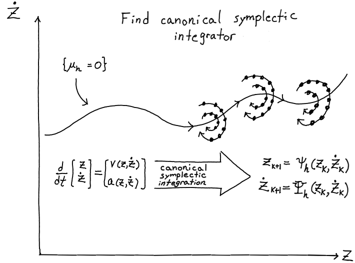
N.B.: $V \cdot \omega = \mathbf{d}H$ iff $V = -\mathbb{J}\nabla H$.

$\mu = 0$ dynamics approximates original system



Part II: Time discretization of symplectic Lorentz system



It is easy to satisfy the frozen-flux condition for Ω, even though ω presented difficulties

Prop. (symplectic maps for symplectic Lorentz system)

If $F : (Z, V) \mapsto (\overline{Z}, \overline{V})$ satisfies

$$\theta_i(\overline{Z}) + \epsilon\, g_{ij}(\overline{Z})\, \overline{V}^j = \partial_{\overline{Z}^i} S(Z, \overline{Z})$$
$$\theta_i(Z) + \epsilon\, g_{ij}(Z)\, V^j = -\partial_{Z^i} S(Z, \overline{Z})$$

for some $S(Z, \overline{Z})$, then Ω is frozen into F.

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for some $S(Z, \overline{Z})$, then Ω is frozen into F.

Doubling dimension made constructing symplectic maps easy!

Where do we get S?

Symplectic Lorentz system can be integrated with help of Hamilton-Jacobi theory

$$L(Z, \dot{Z}) = \underbrace{\frac{1}{2}\epsilon g(\dot{Z}, \dot{Z}) + \theta_i(Z)\dot{Z}^i - H(Z)}_{\text{Lagrangian for symplectic Lorentz system}}$$

Symplectic Lorentz system can be integrated with help of Hamilton-Jacobi theory

$$L(Z, \dot{Z}) = \tfrac{1}{2}\epsilon g(\dot{Z}, \dot{Z}) + \theta_i(Z)\dot{Z}^i - H(Z)$$

$$S(Z, \overline{Z}) = \int_0^{\hbar} L(Z(t), \dot{Z}(t))\, dt$$

$Z(t)$ solves EL equations w/ $(Z(0), Z(\hbar)) = (Z, \overline{Z})$

J. E. Marsden and M. West, *Acta Numerica* **10**: 357–514 (2001)

Symplectic Lorentz system can be integrated with help of Hamilton-Jacobi theory

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this S generates $t=\hbar$ flow of symplectic Lorentz system

Symplectic Lorentz system can be integrated with help of Hamilton-Jacobi theory

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we should approximate this integral

J. E. Marsden and M. West, *Acta Numerica* **10**: 357–514 (2001)

We have derived a useful approximation

Thm.

With $N \gg 1$, $\quad \theta_0/2\pi \notin \mathbb{Q}$, and

$$\hbar = \frac{1}{(2\pi N + \theta_0)}, \quad \epsilon = \frac{1}{(2\pi N + \theta_0)^2},$$

$$\begin{aligned} S(Z, \overline{Z}) = & \int_Z^{\overline{Z}} \vartheta - \hbar H(x) + \hbar^2 g_x(X_H(x), \xi) \\ & - \frac{1}{12} \hbar^2 \partial_k \omega_{j\ell}(x)\, X_H^k(x)\, X_H^j(x)\, \xi^\ell \\ & - \frac{1}{4} \left(\frac{\sin\theta_0}{1 - \cos\theta_0} \right) g_x(\xi - \hbar\, X_H(x), \xi - \hbar\, X_H(x)) \\ & x = (Z + \overline{Z})/2, \quad \xi = \overline{Z} - Z, \end{aligned}$$

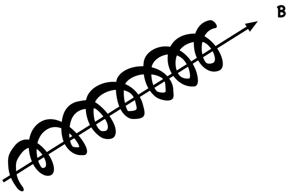
agrees with Jacobi's solution to second-order in $\hbar$.

Why these choices for $\hbar$ and ϵ?

Symplectic Lorentz system

$$\frac{dZ}{dt} = V, \quad \epsilon \frac{DV}{dt} = \mathbb{J}V - \nabla H$$

$$\Downarrow$$

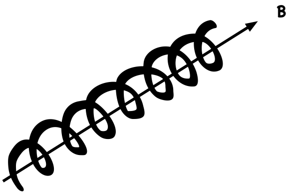


SL system oscillates rapidly on $O(\epsilon)$ timescale

Symplectic Lorentz system

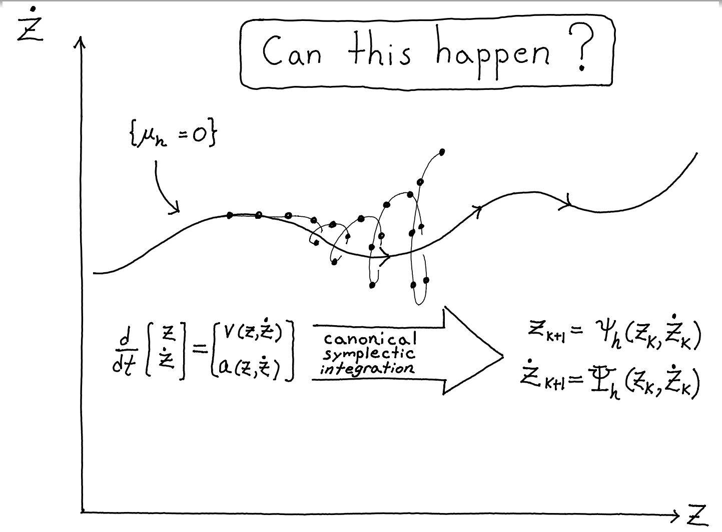
$$\frac{dZ}{dt} = V, \quad \epsilon \frac{DV}{dt} = \mathbb{J}V - \nabla H$$

$$\Downarrow$$



We don't want to resolve these oscillations!

$\hbar = (2\pi N + \theta_0)^{-1}$ is chosen to ensure stability



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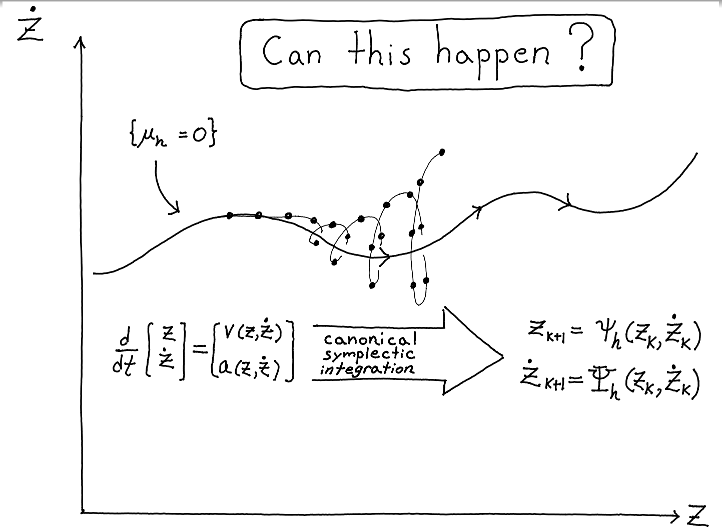
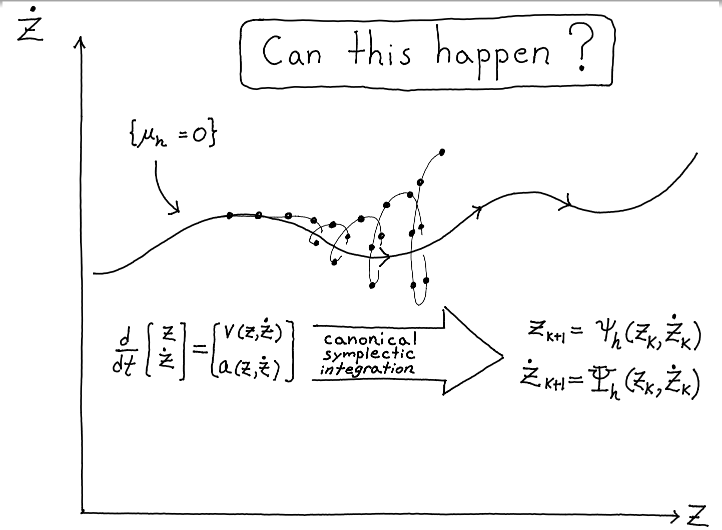


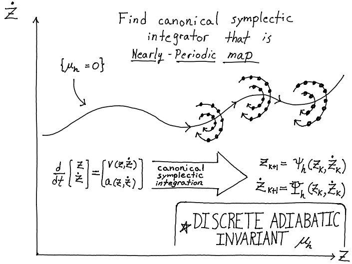
This choice of $\hbar$ ensures answer is **NO** over very large time intervals

$\hbar = (2\pi N + \theta_0)^{-1}$ is chosen to ensure stability



To understand why, we need some more theory...

Part III: Nearly-periodic maps



Nearly-periodic maps are closely related to $U(1)$ actions

Def. (circle action)

A $U(1)$ **action** on a manifold M is a 1-parameter map $\Phi_\theta : M \to M$ such that

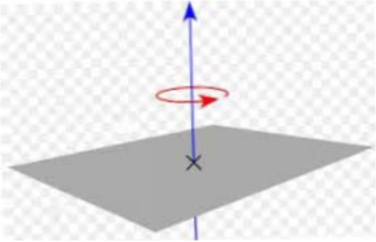
- $\Phi_0 = \Phi_{2\pi} = \mathrm{id}_M$
- $\Phi_{\theta_1+\theta_2} = \Phi_{\theta_1} \circ \Phi_{\theta_2}$

Example 1: **translation along S^1**

Let $M = S^1 = \mathbb{R} \bmod 2\pi$. Typical point $\zeta \in S^1$

$$\Phi_\theta(\zeta) = \zeta + \theta$$

Example 2: **rotation about fixed axis in $\mathbb{R}^3$**



$$\Phi_\theta(\boldsymbol{x}) = (\boldsymbol{e}_z \cdot \boldsymbol{x})\, \boldsymbol{e}_z + \cos\theta\, (\boldsymbol{e}_z \times \boldsymbol{x}) \times \boldsymbol{e}_z + \sin\theta\, \boldsymbol{e}_z \times \boldsymbol{x}$$

Nearly-periodic maps limit to rotations along $U(1)$ actions

Definition 4: (nearly-periodic map)

A mapping $F_\gamma : Z \to Z$ with vector parameter γ is a **nearly-periodic map** if there is a $U(1)$-action $\Phi_\theta : Z \to Z$ and an angle $\theta_0 \in U(1)$ such that

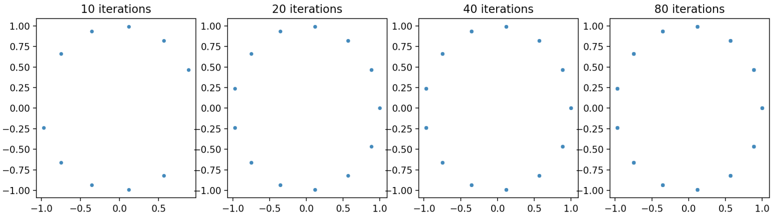
$$F_0 = \Phi_{\theta_0}.$$

If $\theta_0/(2\pi)$ is rational, F_γ is **resonant**. Otherwise it is **non-resonant**.

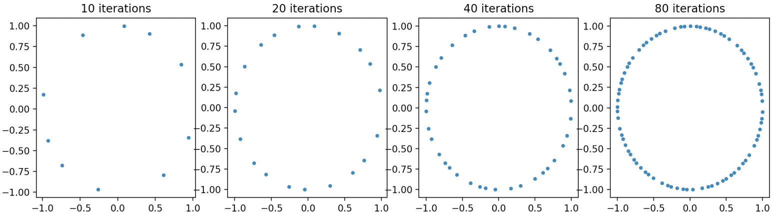
Important class of examples:

If $L_\gamma : Z \to Z$ satisfies $L_0 = \mathrm{id}_Z$ then $F_\gamma = L_\gamma \circ \Phi_{\theta_0}$ is nearly-periodic.

$$\theta \mapsto \theta + \theta_0$$



$$\theta_0 = 2\pi(7/13)$$



$$\theta_0 = 2\pi\phi$$

Discrete nearly-periodic structure $\Rightarrow$ discrete-time $U(1)$ symmetry

Theorem 4: (discrete-time all-orders $U(1)$ symmetry)

Each non-resonant nearly-periodic map F_γ admits a formal $U(1)$ symmetry. Equivalently, there exists a power-series vector field $R_\epsilon = R_0 + R_1[\gamma] + R_2[\gamma,\gamma] + \dots$ such that

- $R_0 = \partial_\theta \Phi_\theta \mid_{\theta=0}$
- $F_\gamma^* R_\gamma = R_\gamma$
- $\exp(2\pi \mathcal{L}_{R_\gamma}) = \mathrm{id}$

Discrete nearly-periodic structure $\Rightarrow$ discrete-time $U(1)$ symmetry

Corollary: (discrete-time adiabatic invariance)

If a non-resonant nearly-periodic map is also Hamiltonian* then it admits an adiabatic invariant. Equivalently, there exists a power series scalar function $\mu_\gamma = \mu_0 + \mu_1[\gamma] + \mu_2[\gamma, \gamma] + \dots$ such that

$$\mu_\gamma(F_\gamma(z)) - \mu_\gamma(z) = 0$$

to all orders in γ for each $z \in Z$.

Proposition.

Our integrator is symplectic nearly-periodic.
See **arXiv:2112.08527** (submitted to JNLS) for details

properties of symplectic Lorentz map

- Symplectic on (Z, V)-space.
  - Flux tensor: $\Omega = \omega + \hbar^2 \Omega_0$

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- Symplectic on (Z, V)-space.
  - Flux tensor: $\Omega = \omega + \hbar^2\,\Omega_0$
- Non-resonant nearly-periodic map
- Has a discrete-time **adiabatic invariant**:
  - $\mu(Z, V) = \frac{1}{2}\,g(V + \mathbb{J}\nabla H, V + \mathbb{J}\nabla H)$

Thm. (discrete-time adiabatic invariance)

For each non-negative $k \in \mathbb{Z}$

$$|\mu(n\hbar) - \mu(0)| = O(\epsilon), \quad n\hbar \in [0, C_k/\epsilon^k]$$

JWB, E. Hirvijoki, M. Leok *In Preparation* (2021)

properties of symplectic Lorentz map

- Symplectic on (Z, V)-space.
- Non-resonant nearly-periodic map
- Has a discrete-time **adiabatic invariant**:
- Enjoys **persistent approximation property**

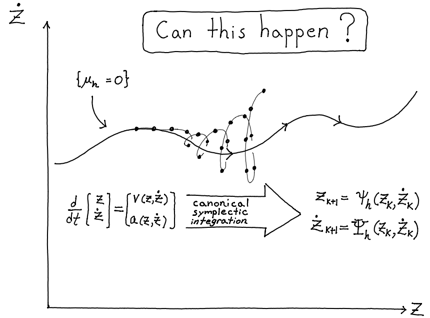
Thm. (Persistent approximation property)

Let C be a compact set and let $(Z, V_\hbar) \in C$ be a smooth $\hbar$-dependent point in C that is positively-contained for each $\hbar$. Also assume $V_\hbar = X_H(Z) + O(\hbar^{1/2})$. For each $N > 0$ there is an integer $k^*(\hbar, N) = O(\hbar^{-N})$ such that

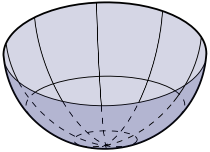
$$Z^{k+1} = Z^k + \hbar\, X_H(Z^k) + \frac{1}{2}\hbar^2\, DX_H(Z^k)[X_H(Z^k)] + O(\hbar^{5/2})$$

$$V^{k+1} = X_H(^{k+1}) + O(\hbar^{1/2}),$$

for each $k \in [0, k^*(\hbar, N)]$.



$$\mu(Z, V) = \frac{1}{2}\, g(V + \mathbb{J}\nabla H, V + \mathbb{J}\nabla H)$$



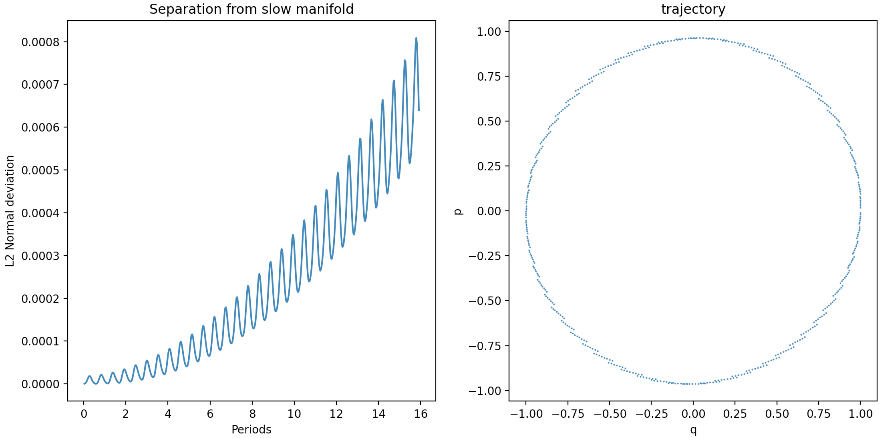
$x^2 + y^2$

(definite)

$\Rightarrow$ Can't wander away from $\mu = 0$ without increasing μ

Dimension doubling without NPM constraint leads to instabilities

Example: "non-canonical pendulum"



C. L. Ellison *et al. Phys. Plasmas* **25**: 052502 (2018).

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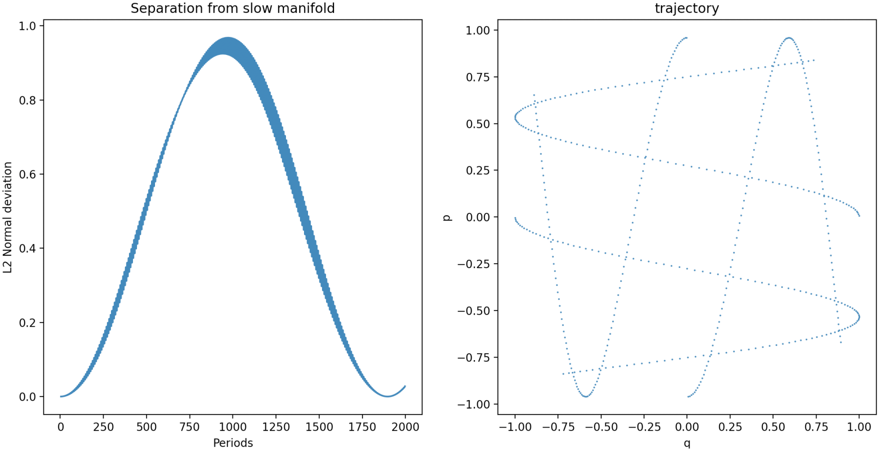
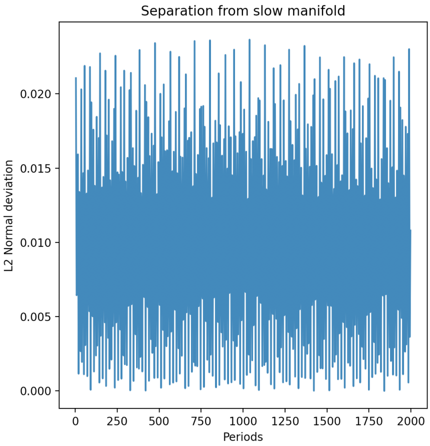
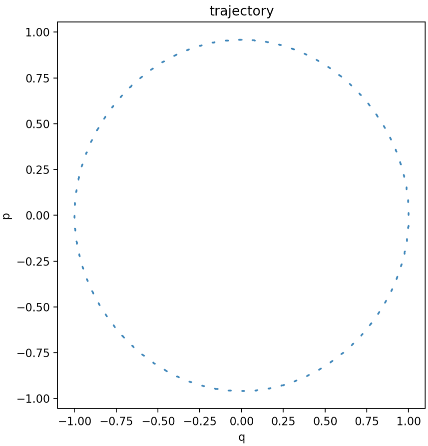


C. L. Ellison *et al.* *Phys. Plasmas* **25**: 052502 (2018).

Instabilities can be eliminated using nearly-periodic maps!

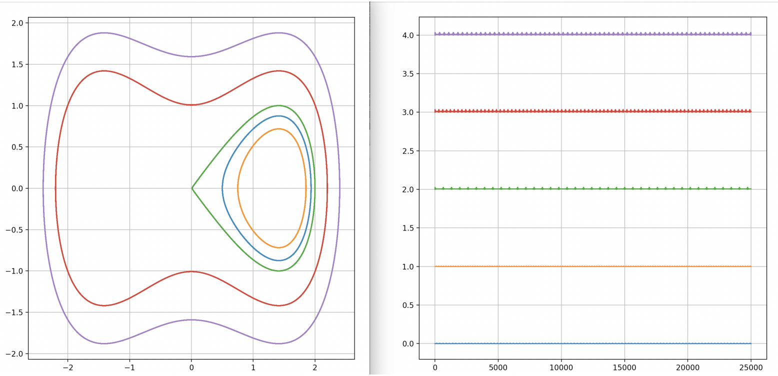




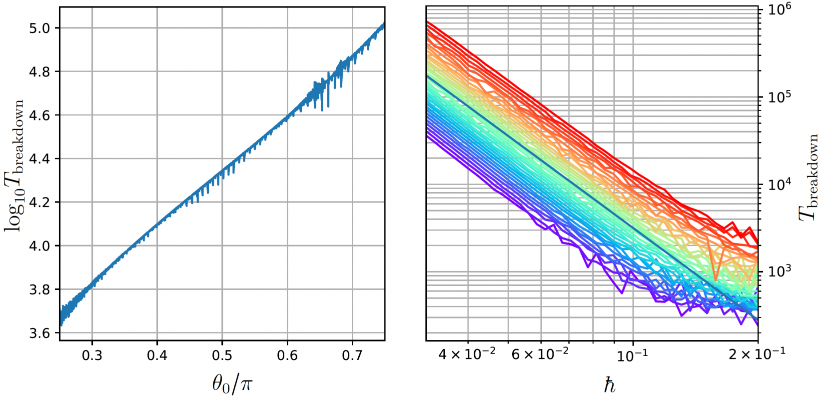
General technique produces new structure-preserving integrator for guiding center dynamics

$$\omega = B(x,y)\, dx \wedge dy, \qquad H = \mu\, B(x,y)$$

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

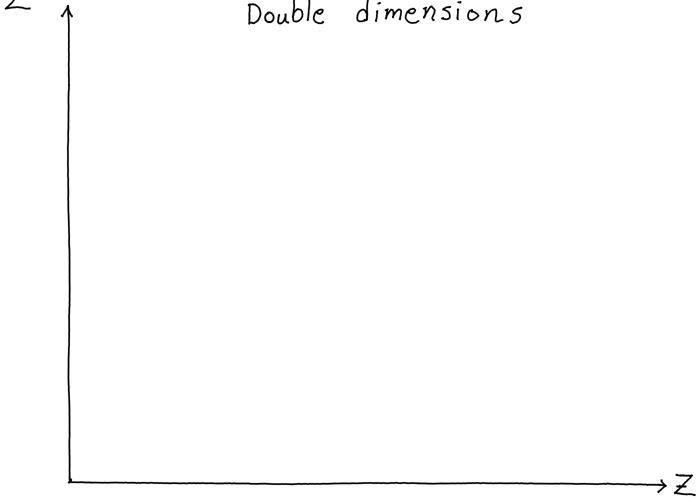


General technique produces new structure-preserving integrator for guiding center dynamics

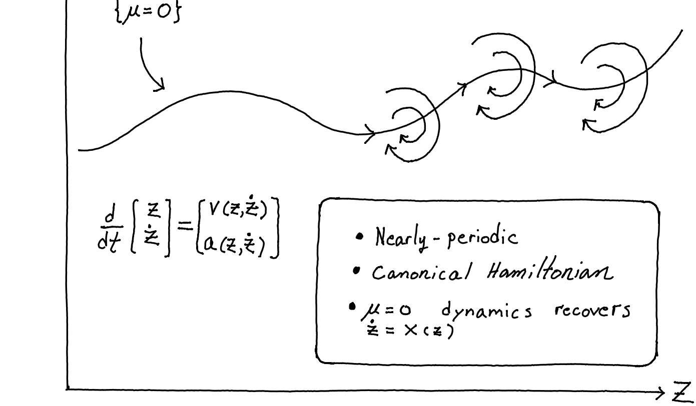


Summary

Double dimensions



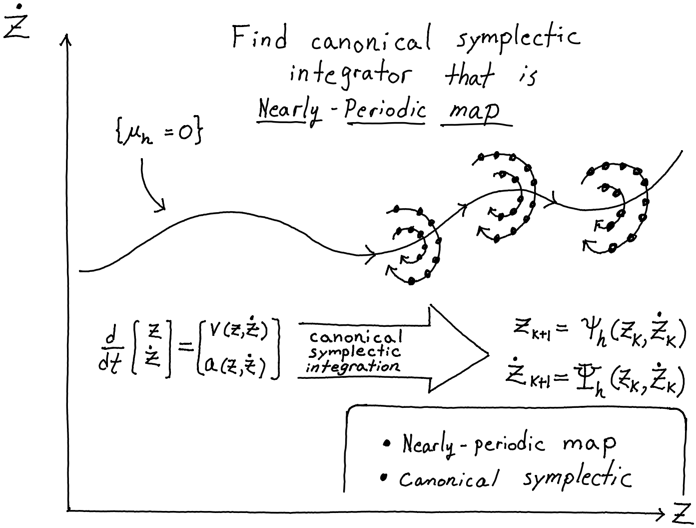
Embed original dynamics
as <u>approximate</u> <u>invariant</u> <u>manifold</u>



$$\frac{d}{dt}\begin{bmatrix} z \\ \dot{z} \end{bmatrix} = \begin{bmatrix} V(z,\dot{z}) \\ a(z,\dot{z}) \end{bmatrix}$$

- Nearly-periodic
- Canonical Hamiltonian
- $\mu = 0$ dynamics recovers $\dot{z} = X(z)$

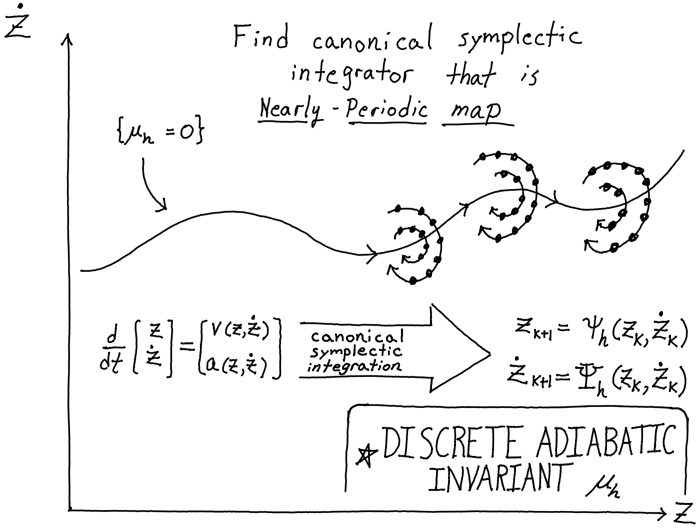
Find canonical symplectic integrator that is <u>Nearly-Periodic</u> <u>map</u>



$$\frac{d}{dt}\begin{bmatrix} Z \\ \dot{Z} \end{bmatrix} = \begin{bmatrix} V(Z,\dot{Z}) \\ a(Z,\dot{Z}) \end{bmatrix} \xrightarrow{\text{canonical symplectic integration}} \begin{aligned} Z_{K+1} &= \Psi_h(Z_K, \dot{Z}_K) \\ \dot{Z}_{K+1} &= \Phi_h(Z_K, \dot{Z}_K) \end{aligned}$$

- Nearly-periodic map
- Canonical symplectic

Find canonical symplectic integrator that is Nearly-Periodic map



$$\frac{d}{dt}\begin{bmatrix} z \\ \dot{z} \end{bmatrix} = \begin{bmatrix} v(z,\dot{z}) \\ a(z,\dot{z}) \end{bmatrix} \xrightarrow{\text{canonical symplectic integration}} \begin{aligned} z_{k+1} &= \Psi_h(z_k, \dot{z}_k) \\ \dot{z}_{k+1} &= \Psi_h(z_k, \dot{z}_k) \end{aligned}$$

$\star$ DISCRETE ADIABATIC INVARIANT μ_h

END