Geometric integration of Hamiltonian systems on exact symplectic manifolds*

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

\[ \mathcal{L}_V \omega = 0 \]

\[ \delta \int_{t_1}^{t_2} L \, dt = 0 \]

N.B.: Steady-state MHD frozen-in law is equivalent to

\[ \mathcal{L}_u (B \cdot dS) = (\nabla \times (B \times u)) \cdot dS = 0. \]
Flux tensor (aka presymplectic form) defines geometry of phase space

<table>
<thead>
<tr>
<th>Euclidean Geometry</th>
<th>PhaseSpace Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Metric tensor: $g_{ij}$</td>
<td>• Flux tensor: $\omega_{ij}$ (presymplectic form)</td>
</tr>
<tr>
<td>• Symmetry: $g_{ij} = g_{ji}$ (measures lengths)</td>
<td>• Skew-Symmetry: $\omega_{ij} = -\omega_{ji}$ (measures areas)</td>
</tr>
<tr>
<td>• No Curvature: $R^\rho_{\sigma\mu\nu} = 0$</td>
<td>• No monopoles: $\partial_i \omega_{jk} + \partial_j \omega_{ki} + \partial_k \omega_{ij} = 0$</td>
</tr>
</tbody>
</table>
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 $\omega_{ij}$ 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.
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

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

1. **Non-degeneracy**: $\omega_{ij}$ invertible
2. **Exactness**: $\omega_{ij} = \partial_j \theta_i - \partial_i \theta_j$
Double dimensions
Embed original dynamics as approximate invariant manifold

\[ \dot{\mathbf{z}} = \begin{bmatrix} \mathbf{V}(\mathbf{z}, \dot{\mathbf{z}}) \\ \mathbf{a}(\mathbf{z}, \dot{\mathbf{z}}) \end{bmatrix} \]

- Nearly-periodic
- Canonical Hamiltonian
- \( \mu = 0 \) dynamics recovers \( \dot{\mathbf{z}} = \mathbf{X}(\mathbf{z}) \)
Find canonical symplectic integrator that is 
**Nearly-Periodic map**

\[
\{\mu_h = 0\}
\]

\[
\frac{d}{dt} \begin{bmatrix} \dot{x} \\ \dot{y} \end{bmatrix} = \begin{bmatrix} V(x,\dot{x}) \\ a(x,\dot{x}) \end{bmatrix}
\]

**Canonical symplectic integration**

\[
\begin{align*}
\chi_{k+1} &= \psi_h(z_k,\dot{z}_k) \\
\dot{z}_{k+1} &= \Phi_h(z_k,\dot{z}_k)
\end{align*}
\]

- **Nearly-periodic map**
- **Canonical symplectic**
Find canonical symplectic integrator that is nearly-periodic map

\[ \mu_h = 0 \]

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

canonical symplectic integration

\[
z_{k+1} = \Psi_h(z_k, \dot{z}_k)
\]

\[
\dot{z}_{k+1} = \Phi_h(z_k, \dot{z}_k)
\]

*DISCRETE ADIABATIC INVARIANT* \[ \mu_h \]
Part I: Symplectic Lorentz embedding

Embed original dynamics as approximate invariant manifold

\[ \dot{z} \]

\[ \begin{bmatrix} y(\tau, \tilde{z}) \\ \alpha(\tilde{z}, \tilde{\tau}) \end{bmatrix} \]

- Nearly periodic
- Canonical Hamiltonian
- \( \mu = 0 \) dynamics recovers
  \( z = x(\tau) \)
Hamilton’s equation has an electromagnetic interpretation

Hamilton’s equation

\[ V^i \omega_{ij} = \partial_j H \]
Hamilton’s equation has an electromagnetic interpretation

Hamilton’s equation

\[ V_i \quad \omega_{ij} = \partial_j H \]

Generator of dynamics
Hamilton’s equation has an electromagnetic interpretation

\[ V^i \omega_{ij} = \partial_j H \]

flux tensor
Hamilton’s equation has an electromagnetic interpretation

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Hamiltonian
Hamilton’s equation has an electromagnetic interpretation.

Hamilton’s equation:

\[ V^i \omega_{ij} = \partial_j H \]

Hamiltonian

Electrostatic field
Hamilton’s equation has an electromagnetic interpretation.

Hamilton’s equation

\[ V^i \omega_{ij} = \partial_j H \]

flux tensor

magnetostatic field
Hamilton’s equation has an electromagnetic interpretation

**Electromagnetic analogue**

\[ \mathbf{v} \times \mathbf{B} = -\mathbf{E} \]
Hamilton’s equation has an electromagnetic interpretation

Electromagnetic analogue

\[ \frac{m}{q} \dot{\mathbf{v}} = \mathbf{E} + \mathbf{v} \times \mathbf{B} \]

Zero-mass limit of Lorentz force
This motivates the study of charged particle motion in these “electromagnetic fields”

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<th>Lorentz force</th>
<th>“Symplectic” Lorentz force</th>
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<td>$E$</td>
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<td>$B$</td>
<td>$\omega$</td>
</tr>
<tr>
<td>$\frac{1}{2} m</td>
<td>\mathbf{v} \rangle^2$</td>
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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 $\omega_{ij}$, a compatible almost complex structure is an almost complex structure $J^i_j$ such that

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

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 $\omega_{ij}$ 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”

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The symplectic Lorentz system parallels the usual Lorentz force law

Original Hamiltonian system

\[ \frac{dZ}{dt} = V(Z), \quad V \cdot \omega = dH \]
The symplectic Lorentz system parallels the usual Lorentz force law

\[ \frac{dZ}{dt} = V, \quad \epsilon \frac{DV}{dt} = J V - \nabla H \]
properties of symplectic Lorentz system

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

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

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

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

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

\( \Rightarrow \text{Periodic because } \mathbb{J}^2 = -1! \)
properties of symplectic Lorentz system

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

**Thm. (adiabatic invariance)**

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

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

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

Corollary:

If $\mu(= \frac{1}{2} g(V + J\nabla H, V + J\nabla H)) = 0$ then $V = -J\nabla H$.

In particular, if $\mu(0) = 0$ then for each $k$

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

N.B.: $V \cdot \omega = dH$ iff $V = -J\nabla H$. 
$\mu = 0$ dynamics approximates original system

Embed original dynamics as approximate invariant manifold

$\dot{\mathbf{z}}$

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

- Nearly-periodic
- Canonical Hamiltonian
- $\mu = 0$ dynamics recovers $\dot{\mathbf{z}} = \mathbf{X}(\mathbf{z})$
Part II: Time discretization of symplectic Lorentz system
It is easy to satisfy the frozen-flux condition for $\Omega$, even though $\omega$ presented difficulties.

**Prop. (symplectic maps for symplectic Lorentz system)**

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

\[
\theta_i(\bar{Z}) + \epsilon g_{ij}(\bar{Z}) \bar{V}^j = \partial_{\bar{Z}i} S(Z, \bar{Z})
\]

\[
\theta_i(Z) + \epsilon g_{ij}(Z) V^j = -\partial_{Zi} S(Z, \bar{Z})
\]

for some $S(Z, \bar{Z})$, then $\Omega$ is frozen into $F$. 
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\theta_i(Z) + \epsilon g_{ij}(Z) V^j = -\partial_Z S(Z, \bar{Z})$

for some $S(Z, \bar{Z})$, then $\Omega$ 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

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

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

\[ L(Z, \dot{Z}) = \frac{1}{2} \epsilon g(\dot{Z}, \dot{Z}) + \theta_i(Z) \dot{Z}_i - H(Z) \]

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

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

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

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\[ S(Z, \overline{Z}) = \int_{0}^{\hbar} L(Z(t), \dot{Z}(t)) \, dt \]

Jacobi’s solution of Hamilton-Jacobi equation

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

this \( S \) generates \( t = \hbar \) flow of symplectic Lorentz system
Symplectic Lorentz system can be integrated with help of Hamilton-Jacobi theory

\begin{align*}
L(Z, \dot{Z}) &= \frac{1}{2} \epsilon g(\dot{Z}, \dot{Z}) + \theta_i(Z) \dot{Z}^i - H(Z) \\
S(Z, \bar{Z}) &= \int_0^\hbar L(Z(t), \dot{Z}(t)) \, dt
\end{align*}

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

we should approximate this integral

We have derived a useful approximation

**Thm.**

With $N \gg 1$, $\theta_0/2\pi \not\in \mathbb{Q}$, and

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

$$
S(Z, \overline{Z}) = \int_{Z}^{\overline{Z}} \varphi - \bar{\hbar}H(x) + \bar{\hbar}^2 g_x(X_H(x), \xi)
$$

$$
- \frac{1}{12} \bar{\hbar}^2 \partial_k \omega_{j\ell}(x) X_H^k(x) X_H^j(x) \xi^\ell
$$

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

$$
x = (Z + \overline{Z})/2, \quad \xi = \overline{Z} - Z,
$$

agrees with Jacobi’s solution to second-order in $\bar{\hbar}$. 
Why these choices for $\hbar$ and $\epsilon$?
$\epsilon = \hbar^2$ ensures fastest timescale is not resolved

**Symplectic Lorentz system**

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

\[\downarrow\]

SL system oscillates rapidly on $O(\epsilon)$ timescale
\[ \epsilon = \hbar^2 \] ensures fastest timescale is not resolved

**Symplectic Lorentz system**

\[
\frac{dZ}{dt} = V, \quad \epsilon \frac{DV}{dt} = \mathcal{J}V - \nabla H
\]

We don’t want to resolve these oscillations!
\[ \hbar = \left(2\pi N + \theta_0\right)^{-1} \] 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

- $\Phi_0 = \Phi_{2\pi} = id_M$
- $\Phi_{\theta_1 + \theta_2} = \Phi_{\theta_1} \circ \Phi_{\theta_2}$
Nearly-periodic maps are closely related to $U(1)$ actions

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

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

$$\Phi_\theta(\zeta) = \zeta + \theta$$
Nearly-periodic maps are closely related to $U(1)$ actions

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

$$
\Phi_\theta(x) = (e_z \cdot x) e_z + \cos \theta (e_z \times x) \times e_z + \sin \theta e_z \times x
$$
Definition 4: (nearly-periodic map)

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

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

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

Important class of examples:

If $L_\gamma : \mathbb{Z} \to \mathbb{Z}$ satisfies $L_0 = \text{id}_\mathbb{Z}$ then $F_\gamma = L_\gamma \circ \Phi_{\theta_0}$ is nearly-periodic.
\[ \theta \mapsto \theta + \theta_0 \]

\[ \theta_0 = 2\pi \left( \frac{7}{13} \right) \]

\[ \theta_0 = 2\pi \phi \]
Theorem 4: (discrete-time all-orders $U(1)$ symmetry)

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

- $R_0 = \partial_\theta \Phi_{\theta} \mid_{\theta=0}$
- $F_\gamma^* R_\gamma = R_\gamma$
- $\exp(2\pi \mathcal{L}_{R_\gamma}) = \text{id}$
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 $\mu_\gamma = \mu_0 + \mu_1[\gamma] + \mu_2[\gamma, \gamma] + \ldots$ such that

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

to all orders in $\gamma$ for each $z \in \mathbb{Z}$. 

* Hamiltonian refers to a system where the Hamiltonian function remains constant in time.
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: \(\Omega = \omega + \hbar^2 \Omega_0\)
properties of symplectic Lorentz map

- Symplectic on \((Z, V)\)-space.
  - Flux tensor: \(\Omega = \omega + \hbar^2 \Omega_0\)
- Non-resonant nearly-periodic map
properties of symplectic Lorentz map

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

**Thm. (discrete-time adiabatic invariance)**

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

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

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 \( k \in [0, k^*(\hbar, N)] \).
\[ \mu(Z, V) = \frac{1}{2} g(V + \mathcal{J} \nabla H, V + \mathcal{J} \nabla H) \]

⇒ Can’t wander away from \( \mu = 0 \) without increasing \( \mu \)
Dimension doubling without NPM constraint leads to instabilities

Example: “non-canonical pendulum”

Dimension doubling without NPM constraint leads to instabilities

Example: “non-canonical pendulum”

Instabilities can be eliminated using nearly-periodic maps!
General technique produces new structure-preserving integrator for guiding center dynamics

\[ \omega = B(x, y) \, dx \wedge dy, \quad H = \mu \, B(x, y) \]

\[ B(x, y) = 2 + y^2 - x^2 + \frac{1}{4}x^4 \]
General technique produces new structure-preserving integrator for guiding center dynamics
Summary
Double dimensions
Embed original dynamics as approximate invariant manifold

\[ \{ \mu = 0 \} \]

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

- Nearly-periodic
- Canonical Hamiltonian
- \( \mu = 0 \) dynamics recovers \( \dot{z} = X(z) \)
Find canonical symplectic integrator that is **Nearly-Periodic** map

\[ \mu_h = 0 \]

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

**canonical symplectic integration**

\[
\mathbf{z}_{k+1} = \mathbf{\Psi}_h (\mathbf{z}_k, \mathbf{\dot{z}}_k)
\]

\[
\mathbf{\dot{z}}_{k+1} = \mathbf{\Phi}_h (\mathbf{z}_k, \mathbf{\dot{z}}_k)
\]

- **Nearly-periodic map**
- **Canonical symplectic**
Find canonical symplectic integrator that is Nearly-Periodic map

\[ \{ \mu_n = 0 \} \]

\[ \frac{d}{dt} \begin{bmatrix} \dot{z} \\ \dot{\dot{z}} \end{bmatrix} = \begin{bmatrix} V(z, \dot{z}) \\ a(z, \dot{z}) \end{bmatrix} \] canonical symplectic integration

\[ z_{k+1} = \Psi_h(z_k, \dot{z}_k) \]

\[ \dot{z}_{k+1} = \Phi_h(z_k, \dot{z}_k) \]

**DISCRETE ADIABATIC INARIANT**  
\[ \mu_h \]
END