Island myriads in periodic potentials

Matheus Lazarotto

Iberê Caldas

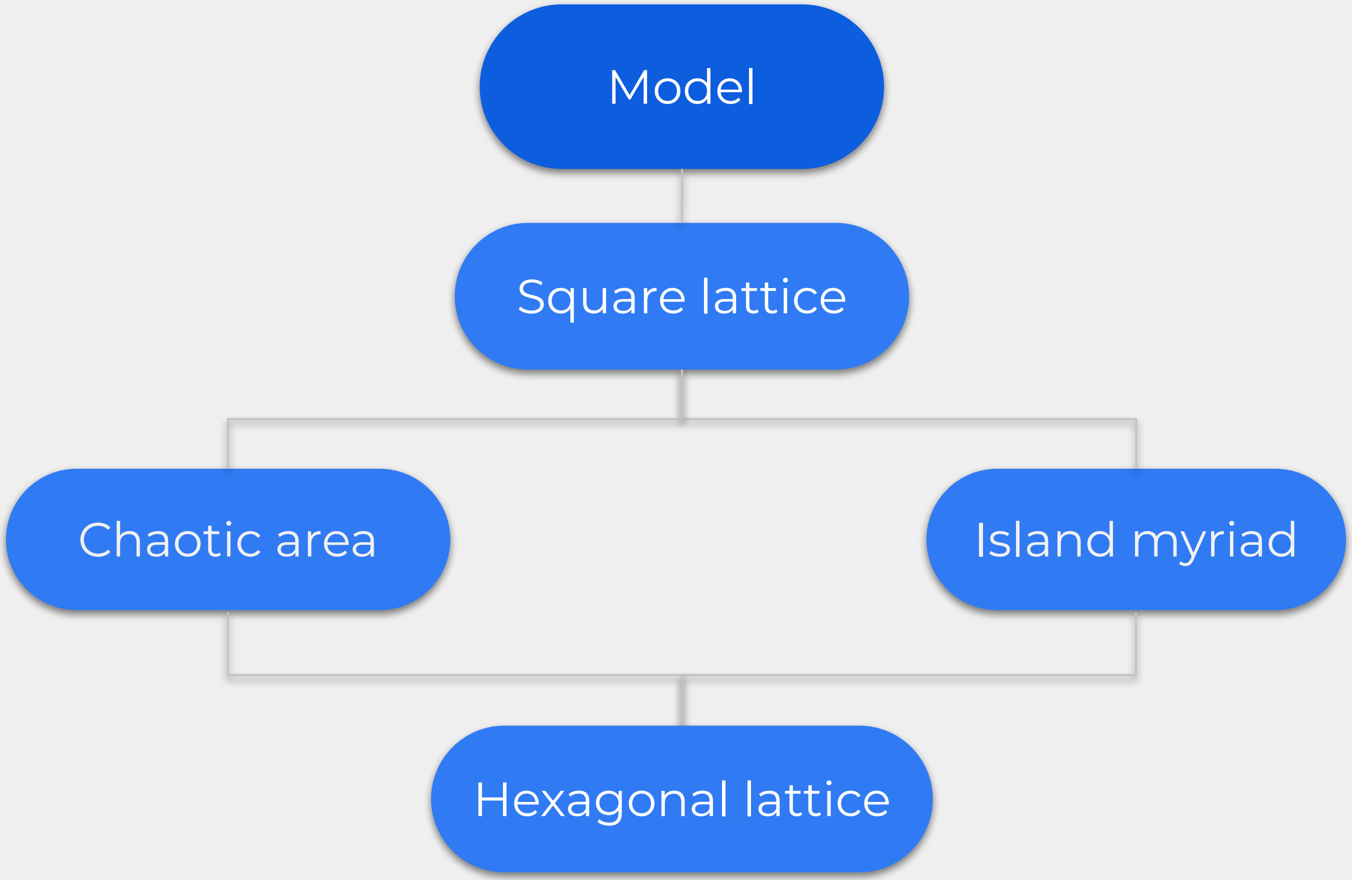
Yves Elskens

PGF5005 - Mecânica Clássica

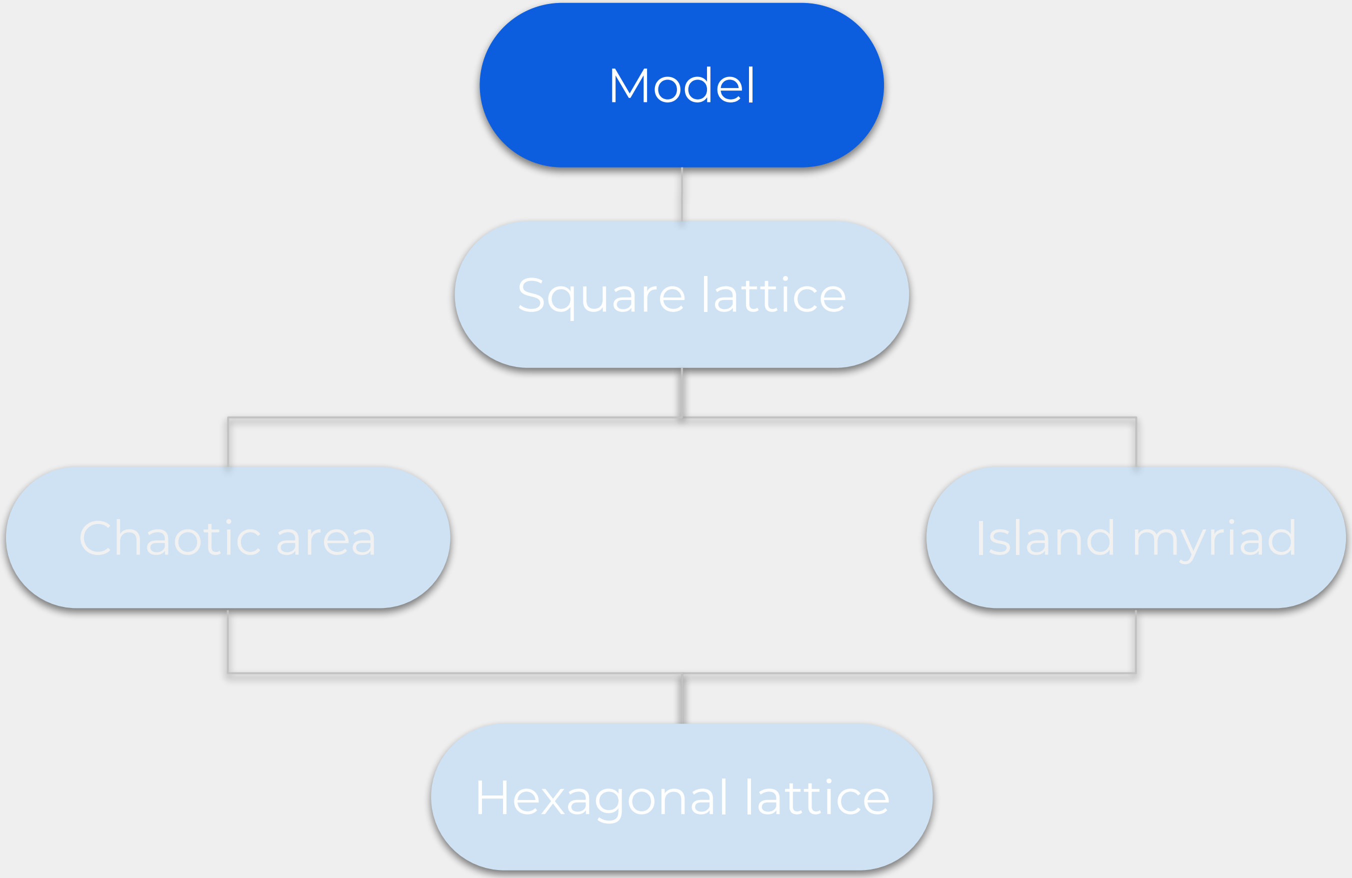
Segundo semestre – 2025

Oscillations Control Group

Summary


Model
Square lattice
Chaotic area
Island myriad
Hexagonal lattice

Summary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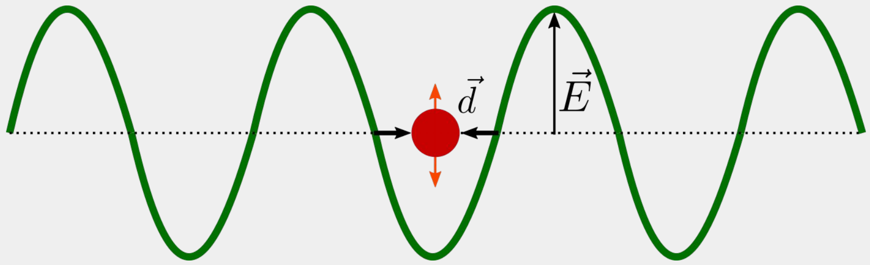
Optical lattices

- Dipole induction in neutral atoms via a laser electrical field

$$\vec{d}(t) = \rho(\omega)\vec{E}(\vec{r},t)$$



- Average interaction potential[1]

$$V_{\text{dip}} = -\langle \vec{d}(t) \cdot \vec{E}(\vec{r},t) \rangle$$

$$V_{\text{dip}} = -\frac{1}{2}\rho(\omega)|\vec{E}(\vec{r})|^2$$

- Restoring force trapping particles in wave minima

$$\vec{F}_{\text{dip}} = \frac{1}{2}\rho(\omega)\vec{\nabla}|\vec{E}(\vec{r})|^2$$

[1] R. Grimm *et al.* Advances in Atomic, Molecular and Optical Physics **42** (2000)

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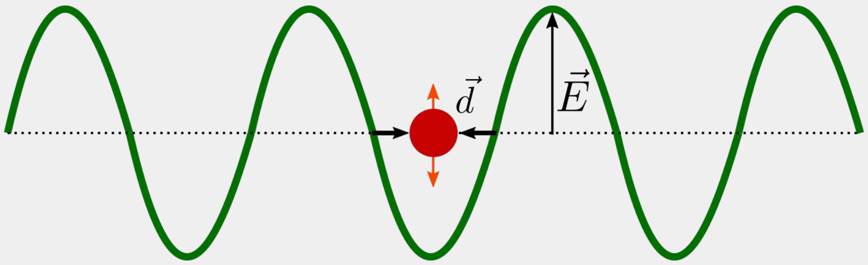

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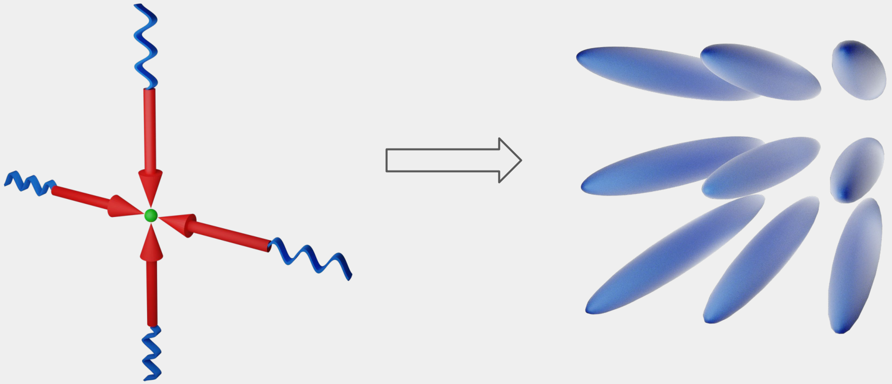
- Superposition of orthogonal beams in **2D** (cigar-shaped cells[1])



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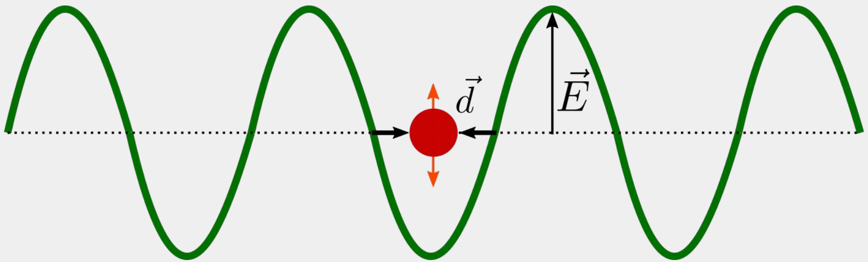

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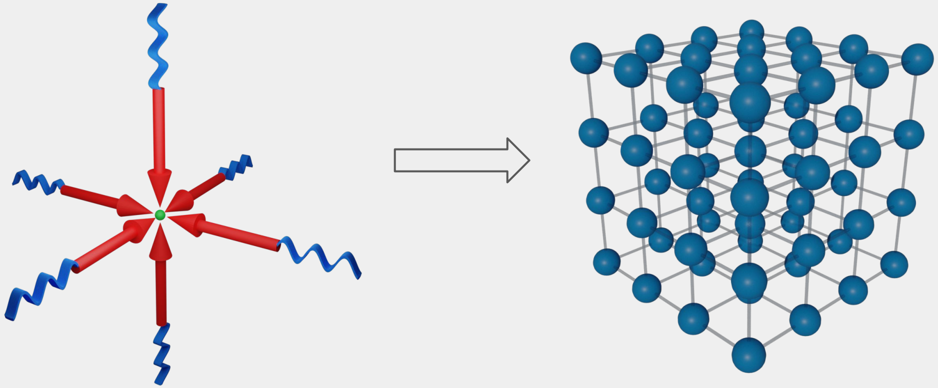
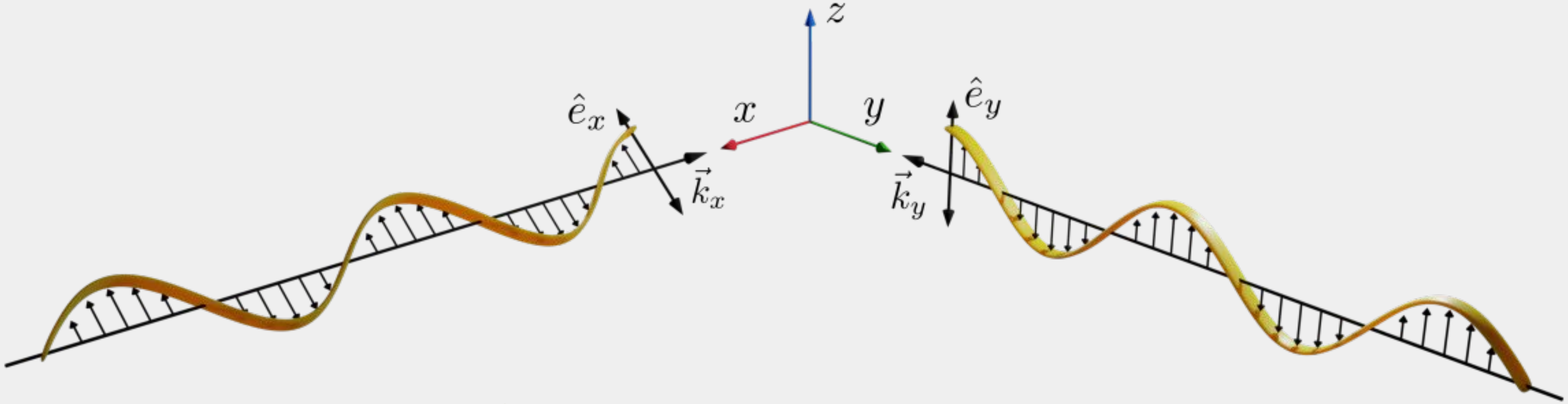
- Superposition of orthogonal beams in **3D** (crystal shaped lattice[1])



[1] R. Grimm *et al.* Advances in Atomic, Molecular and Optical Physics **42** (2000)

Hamiltonian – square lattice

- Superposition of orthogonal waves (**x-y** plane)



- Superposed electrical fields

$$\vec{E}(\vec{r},t) = E_{0x}\cos(k_x x + \phi_x)e^{-i\omega_x t}\,\hat{e}_x + E_{0y}\cos(k_y y + \phi_y)e^{-i\omega_y t}\,\hat{e}_y$$

- Conservative potential (normalized units)

$$V(\vec{r}) = U\left(\cos^2(x) + \cos^2(y) + 2\alpha\cos(x)\cos(y)\right)$$

with laser coupling as $\alpha = \left(\hat{e}_x \cdot \hat{e}_y\right)\cos(\phi_x - \phi_y)$

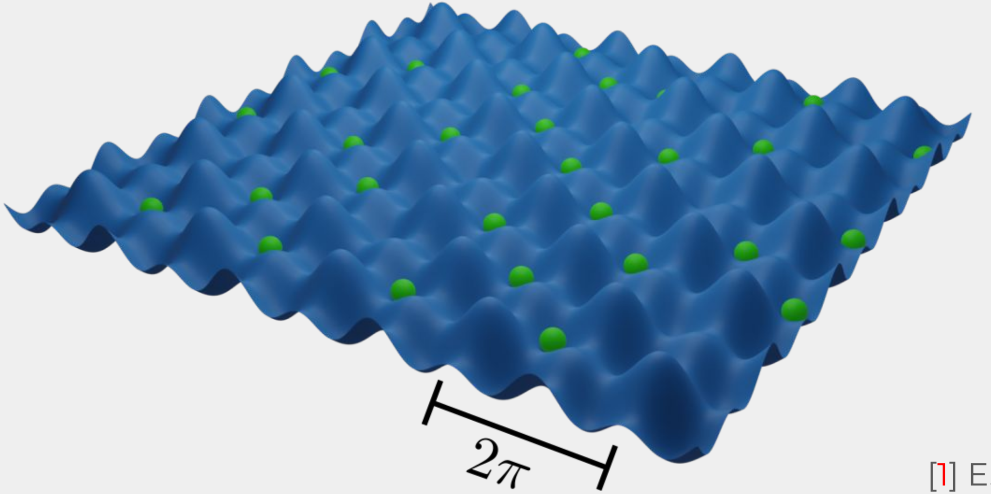
Hamiltonian – square lattice

- Ignoring particles interaction, trajectories are regarded as classical

$$H(x, y, p_x, p_y) = p_x^2 + p_y^2 + V(x, y)$$

where

$$V(x, y) = U\left(\cos^2(x) + \cos^2(y) + 2\alpha\cos(x)\cos(y)\right)$$



- Energy scale (laser intensity)[1]

$$U = 20$$

- Particle energy $H(x, y, p_x, p_y)$

$$E \in [0, V_{\max}]$$

- Wave coupling (perturbation)

$$\alpha \in [0, 1]$$

[1] E. Horsley *et al.* Physical Review E **89** (2014)

Equilibrium points

$$V(x,y) = U\left(\cos^2(x) + \cos^2(y) + 2\alpha\cos(x)\cos(y)\right)$$

- **Global minima**

$$V_{\text{min}} = 0$$

- **Global maxima**

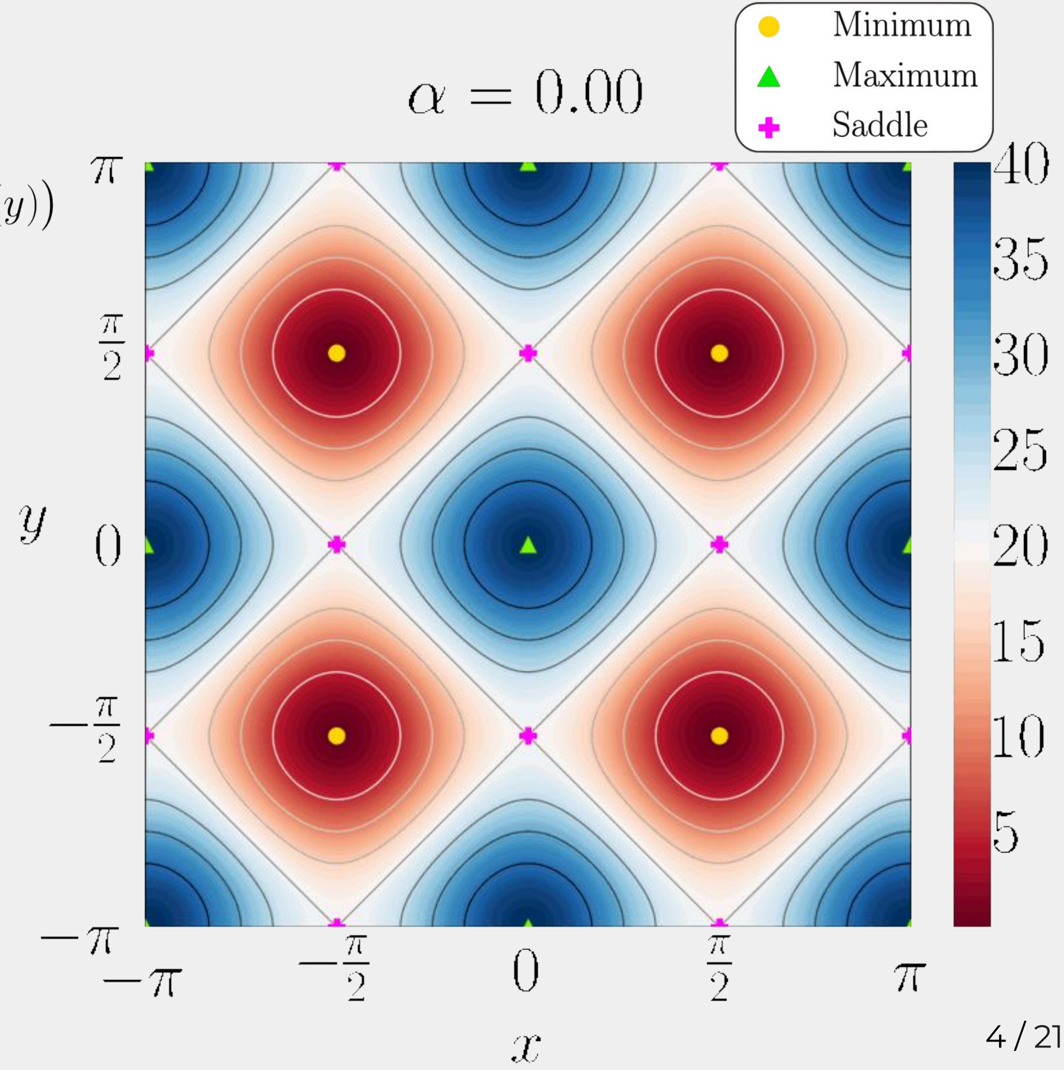
$$V_{\text{g-max}} = 2U(1+\alpha)$$

- **Local maxima**

$$V_{\text{l-max}} = 2U(1-\alpha)$$

- **Saddle**

$$V_{\text{sad}} = U(1-\alpha^2)$$



Symmetries

$$V(x,y) = U\left(\cos^2(x) + \cos^2(y) + 2\alpha\cos(x)\cos(y)\right)$$

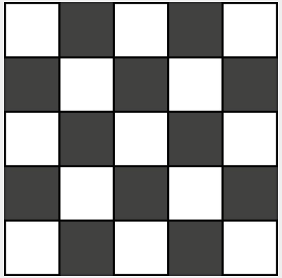
- Symmetric under **rotations**:

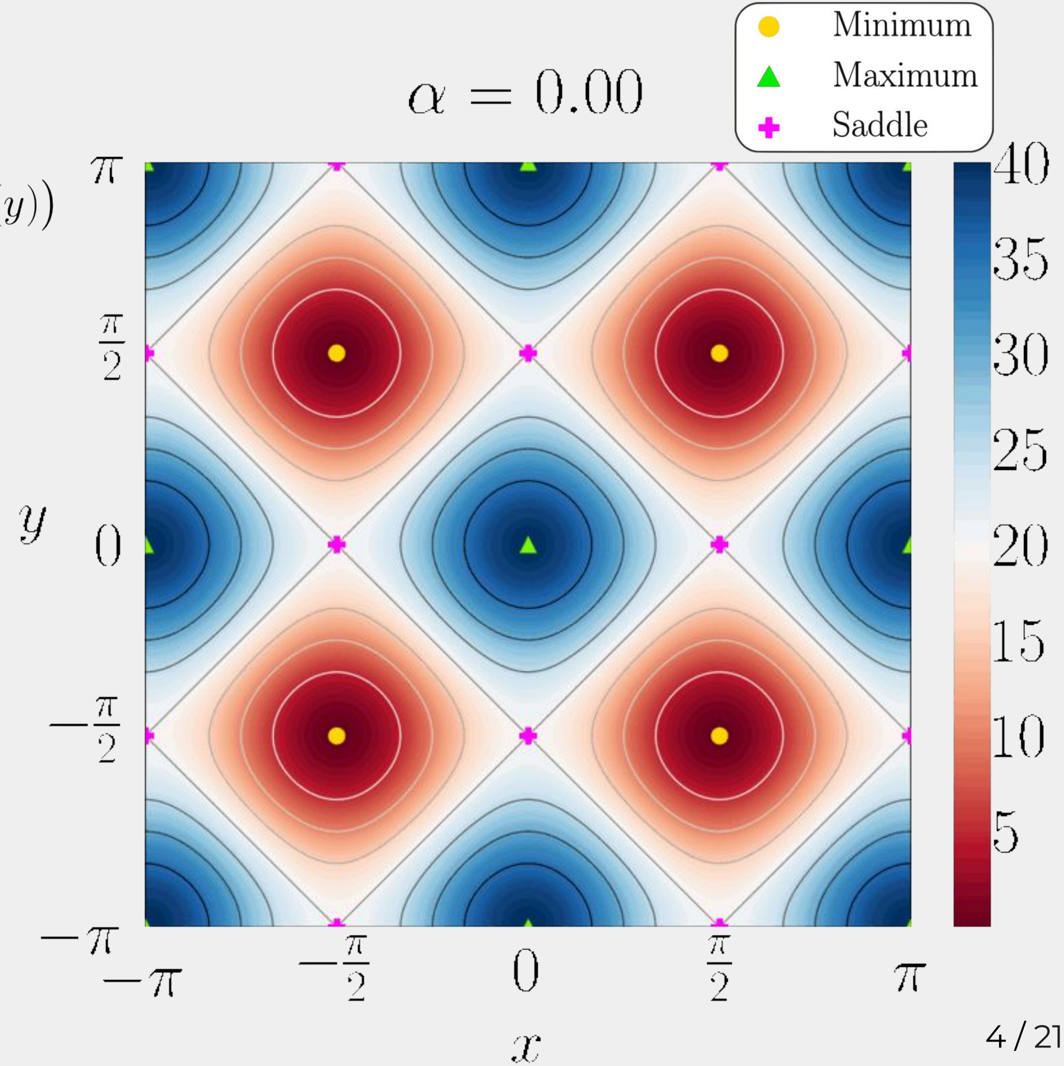
$$\left(\frac{n\pi}{2}, n \in \mathbb{Z}\right)$$

- Symmetric under **translations**:

$$(2m\pi,\ m \in \mathbb{Z})$$

- Square **tiling** symmetry





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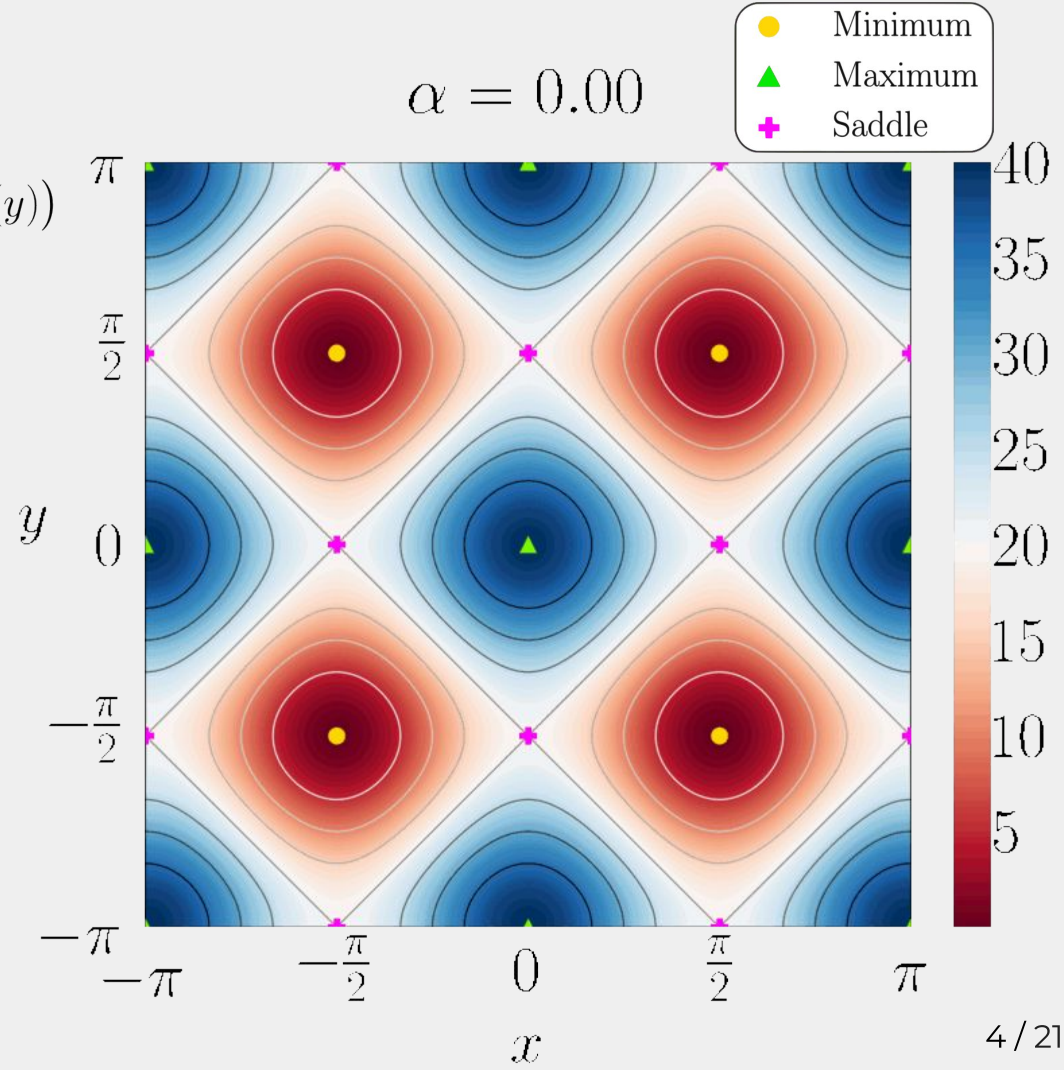
- Dynamical effect of symmetries

Island myriad phenomenon



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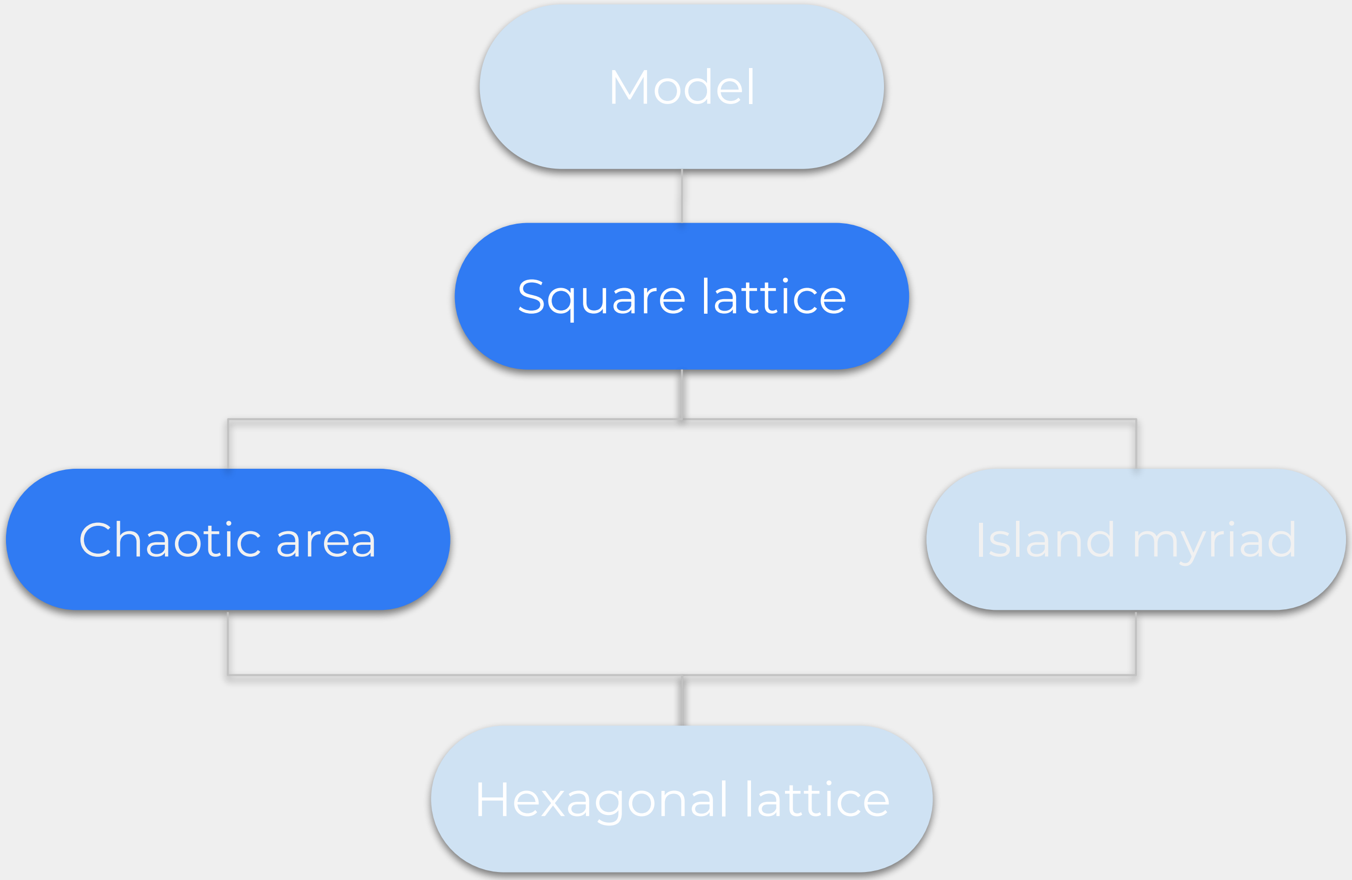
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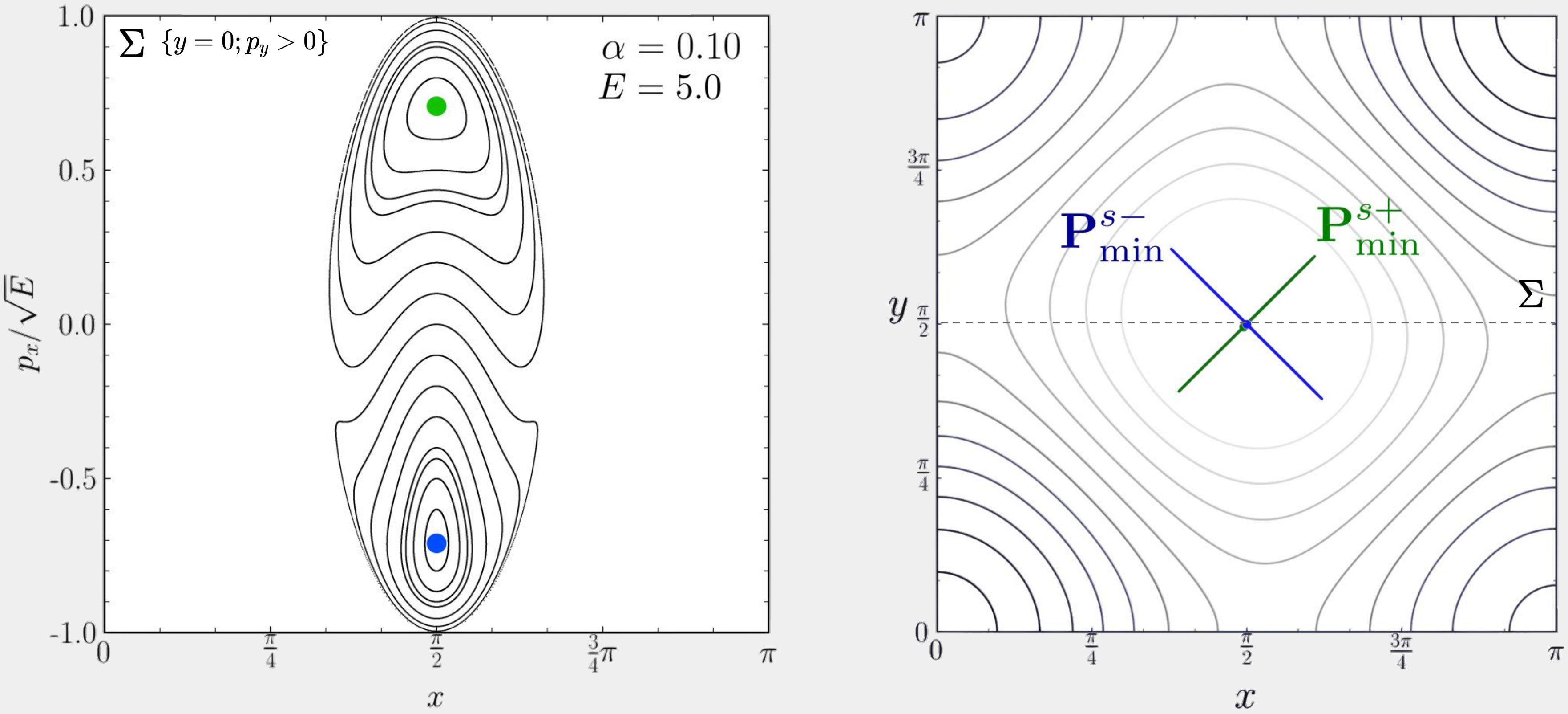
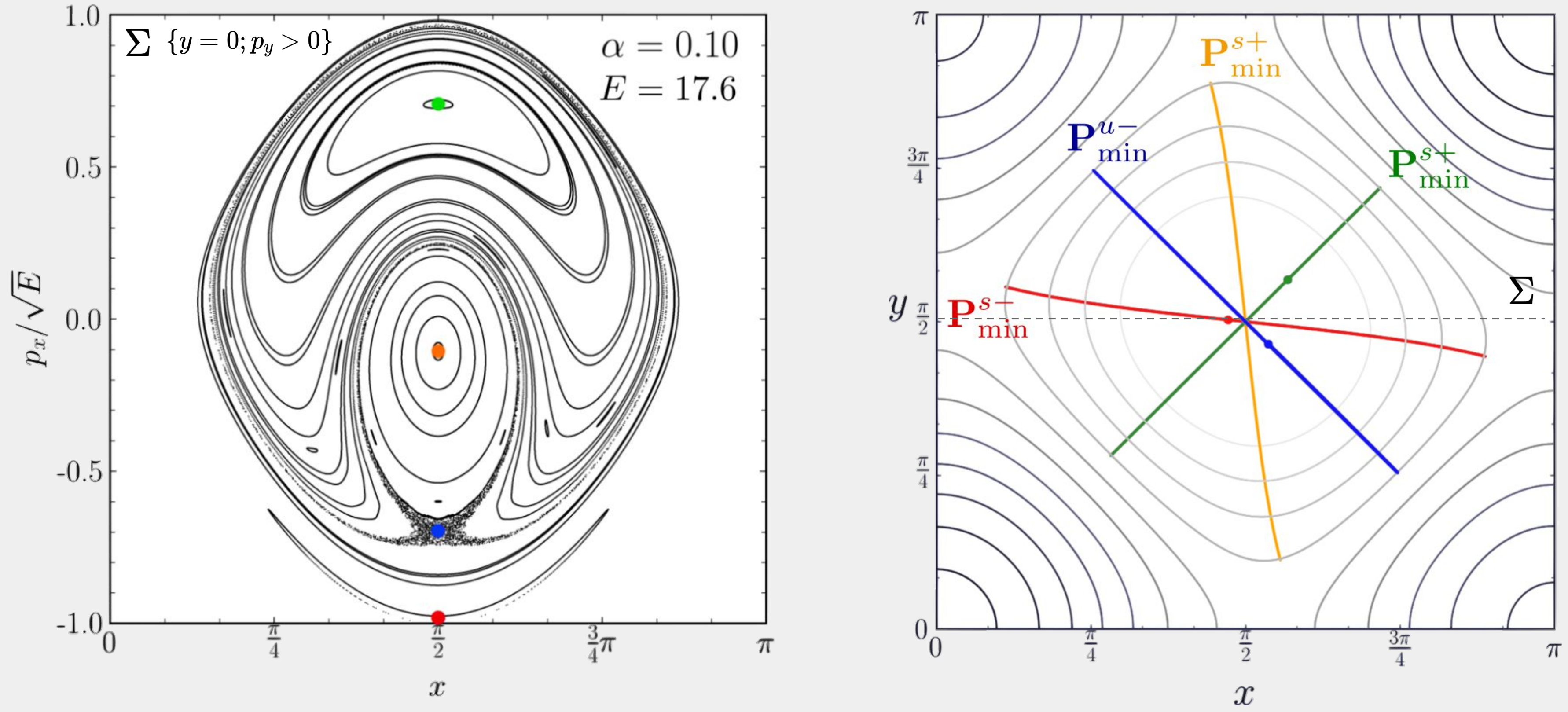
Low energies - Periodic orbit bifurcation



Low energies - Unstable periodic orbit bifurcation



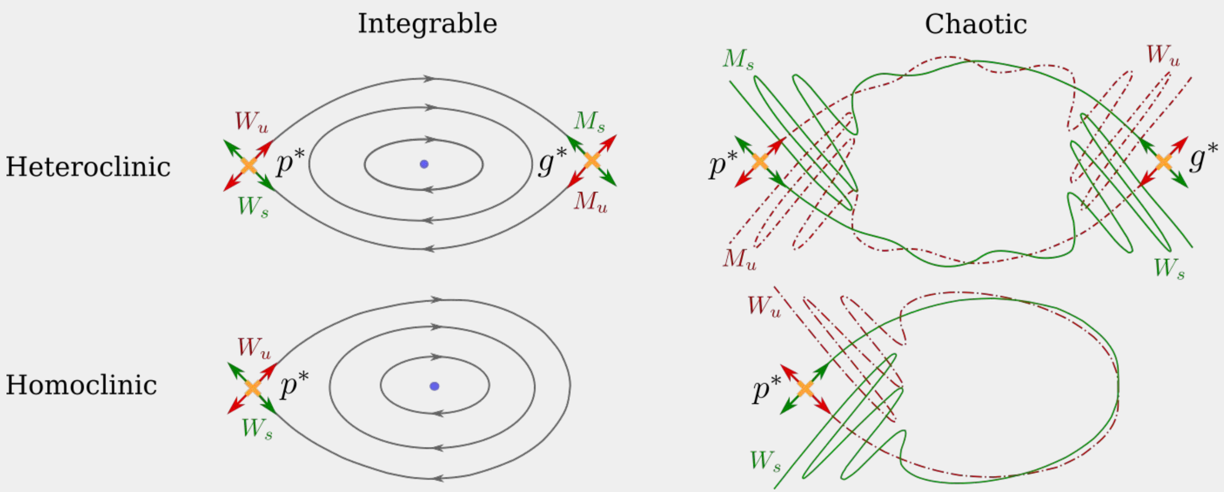
- The stable orbits in red and orange allow for direct diffusion between cells when $E > V_{\text{saddle}}$

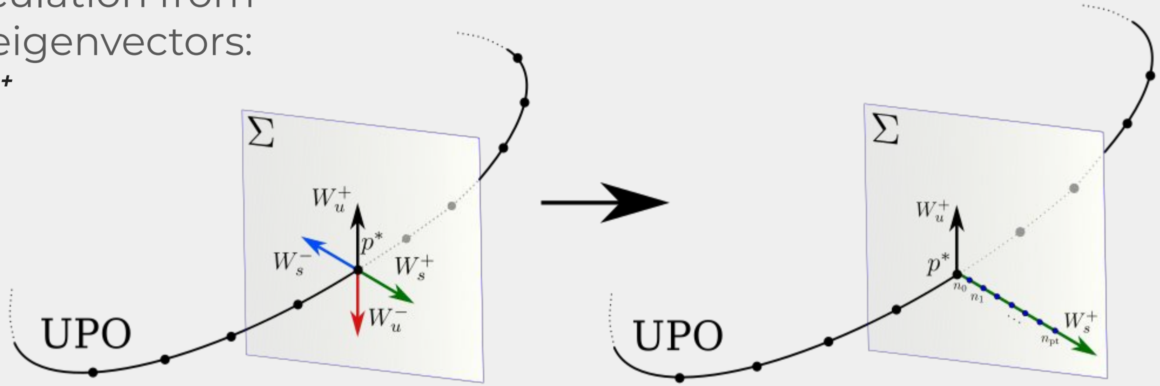
Manifolds

- Disruption of **separatrix** invariant into a chaotic layer

- Infinite tangle between **stable** and **unstable** branches induces chaotic motion, densely filling a 2D area as a fractal

- Numerical calculation from periodic orbit eigenvectors: W_s^+, W_s^-, W_u^-, W_u^+

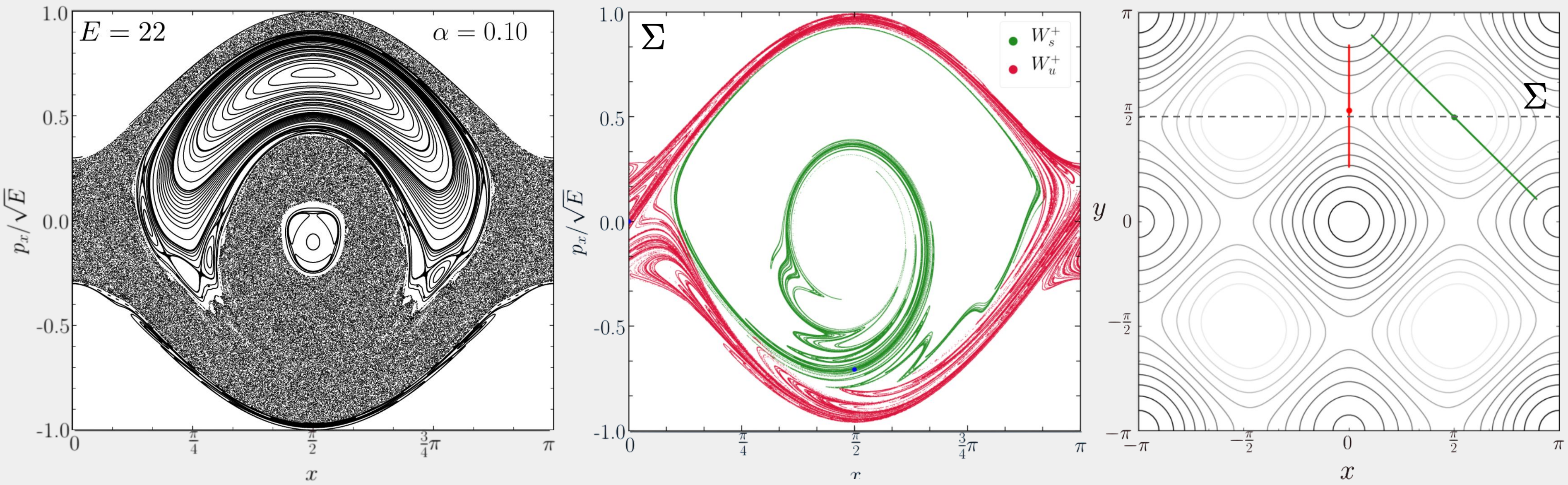




Manifolds for diffusion onset

- Slightly above diffusion onset, manifolds from orbits over saddle points describe the transport of particles between lattice cells.

- Small superposition between the inner (green) and outer (red) layers.



Manifolds for diffusion onset

- Soon after diffusion onset, manifolds from orbits over saddle points describe the transport of particles between lattice cells.

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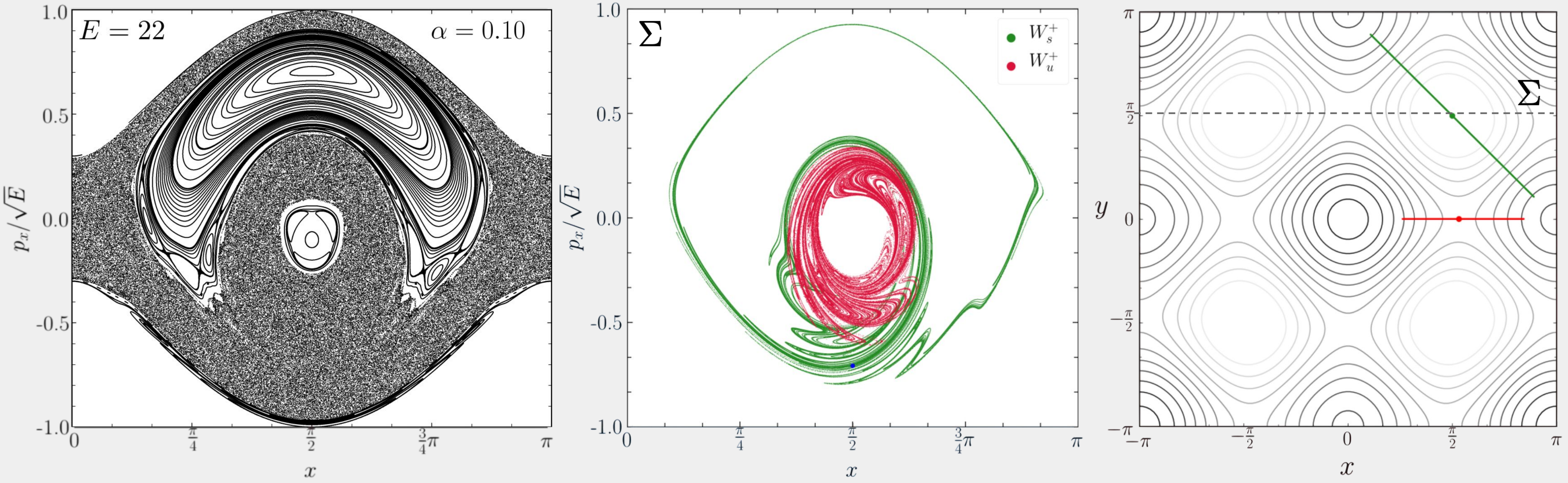


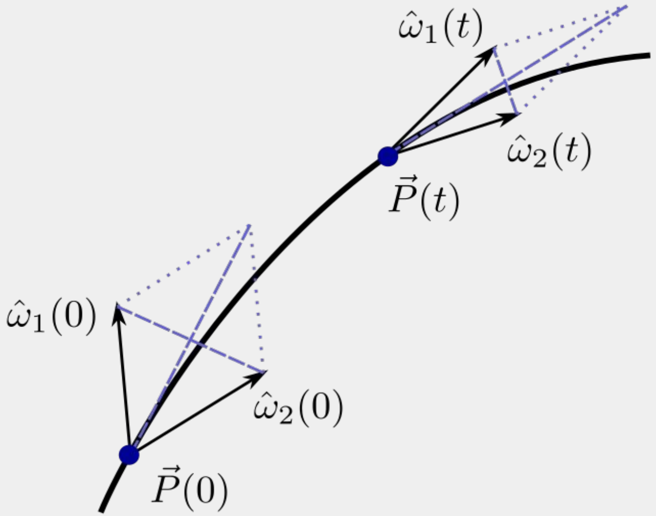
SALI method

- Smaller Alignment Index (SALI)[1]: a quick method for orbits discrimination.

Two deviation vectors $\hat{\omega}_i$ are evolved in tangent space in parallel to an orbit:

$$\mathrm{SALI}(t) = \min\left(||\hat{\omega}_1(t) - \hat{\omega}_2(t)||, ||\hat{\omega}_1(t) + \hat{\omega}_2(t)||\right)$$

- Chaotic case (SALI(t) → 0):



[1] C. Skokos. Journal of Physics A: Mathematical and General **34** (2001)

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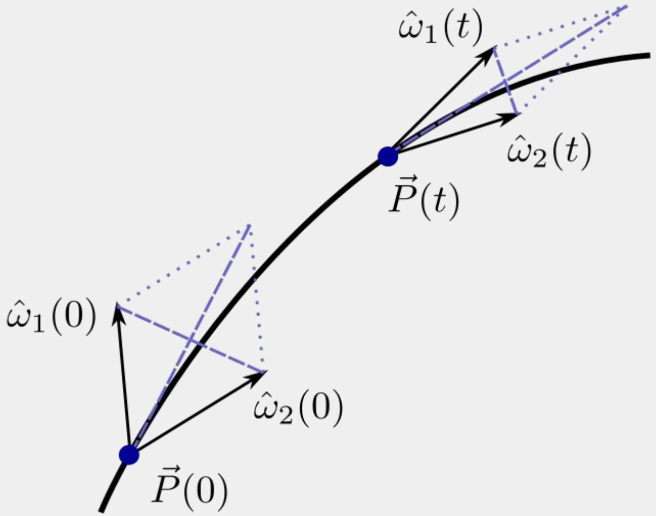
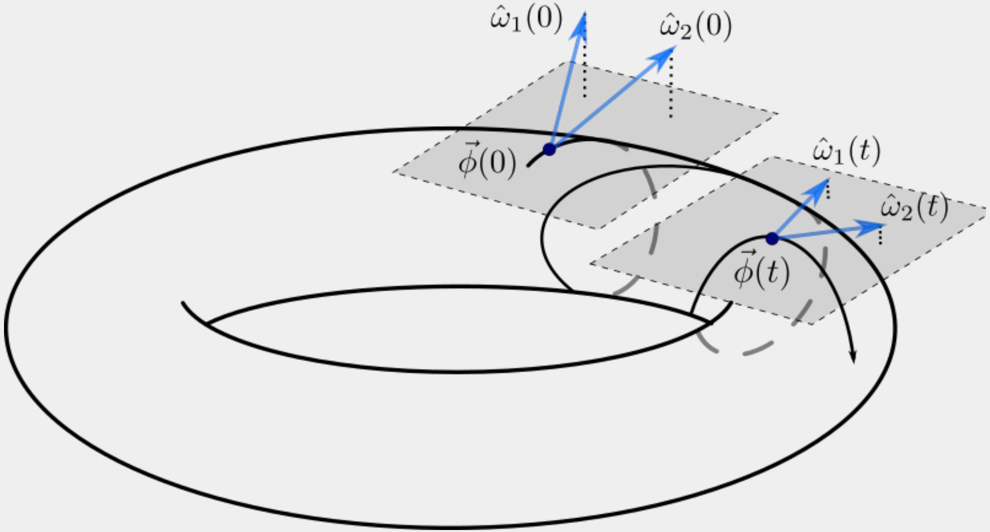


- **Regular case (SALI(t) ≅ cte ≠ 0):**



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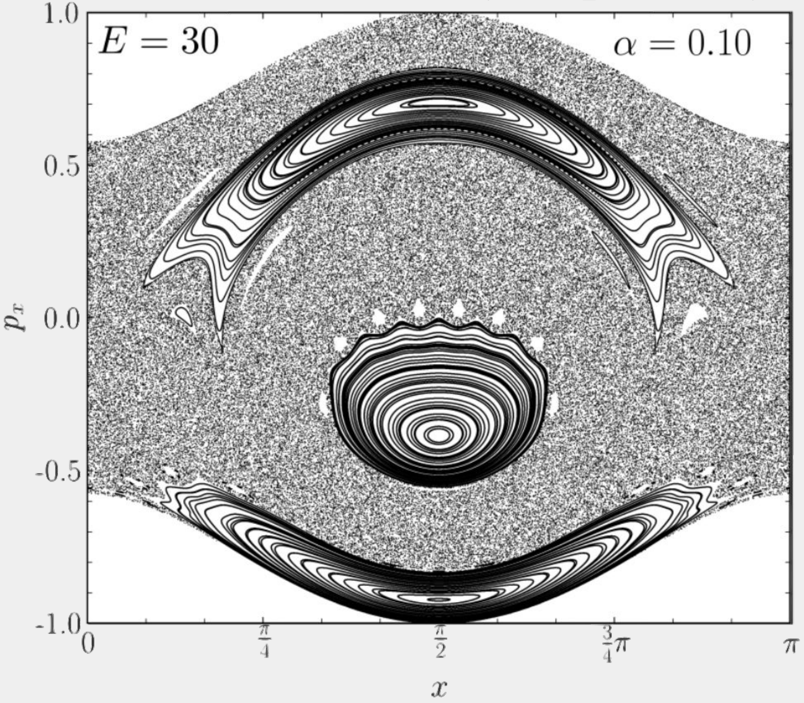
Stability area measurement

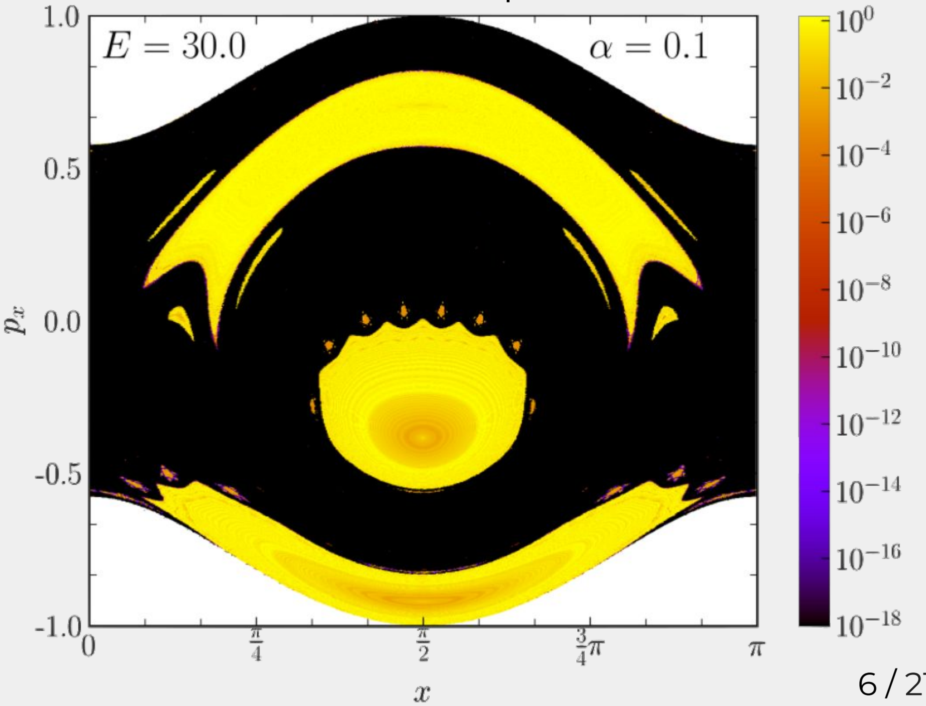
- **Chaotic**/**Regular** areas calculated when summed over a grid mesh

- Analogous to Lyapunov exponent methods but usually with faster convergence

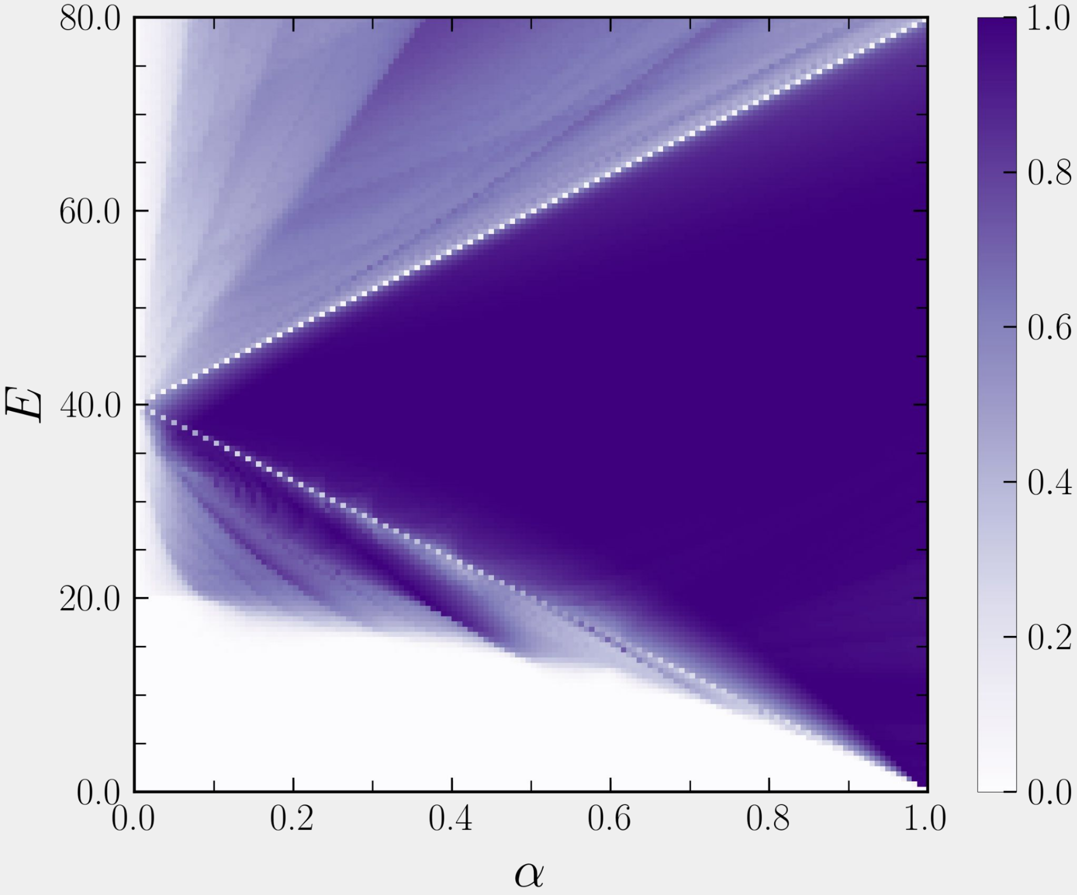
Poincaré Section $\left(y = \frac{\pi}{2}, p_y > 0\right)$



SALI map

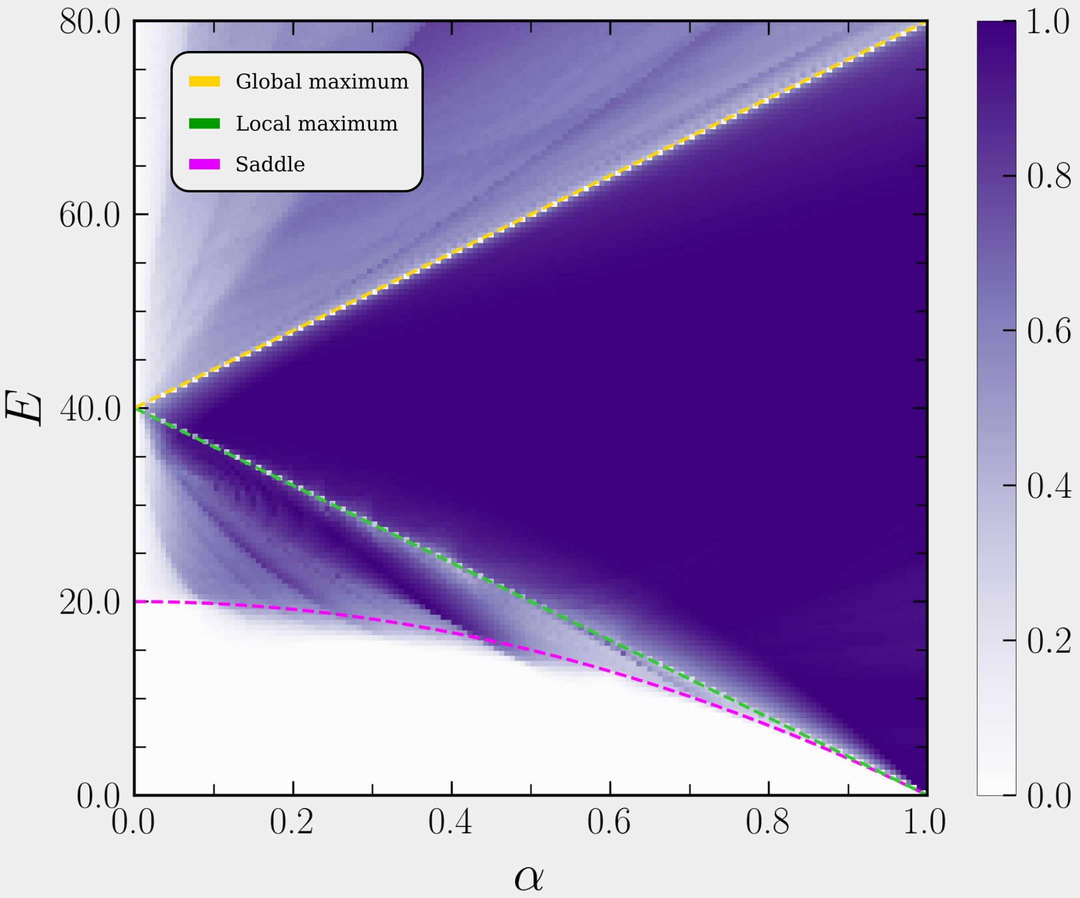


Chaotic area



- Small predominance of chaos for energies below saddle points.
- **Ergodic limit** above the instability lines induced by maxima points.

Chaotic area



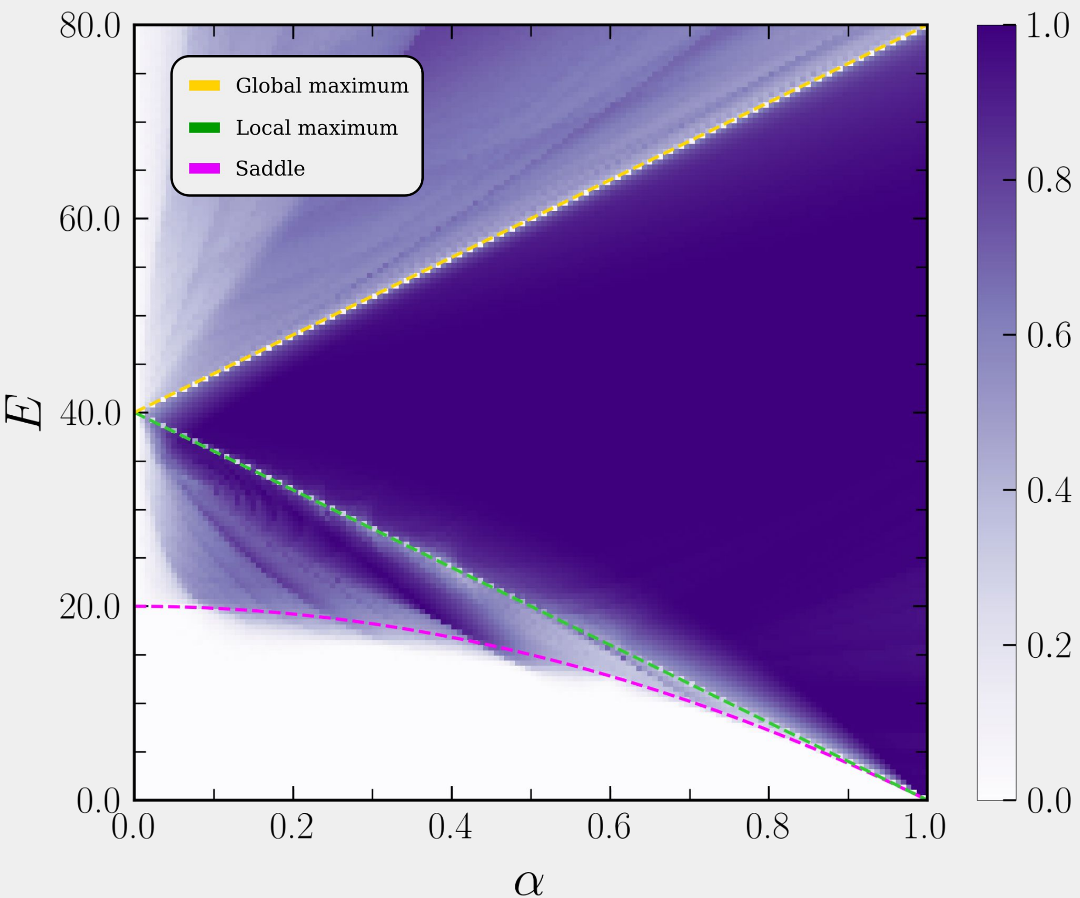
- Small predominance of chaos for energies below saddle points.
- **Ergodic limit** above the instability lines induced by maxima points.
- Emergence of stable structures over **local** and **global** maxima energy lines.

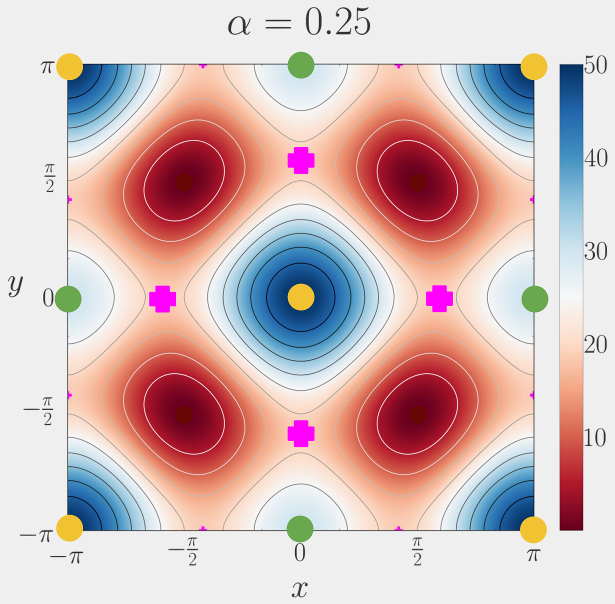
$$V_{\text{g-max}} = 2U(1+\alpha)$$

$$V_{\text{l-max}} = 2U(1-\alpha)$$

$$V_{\text{saddle}} = U(1-\alpha^2)$$

Chaotic area





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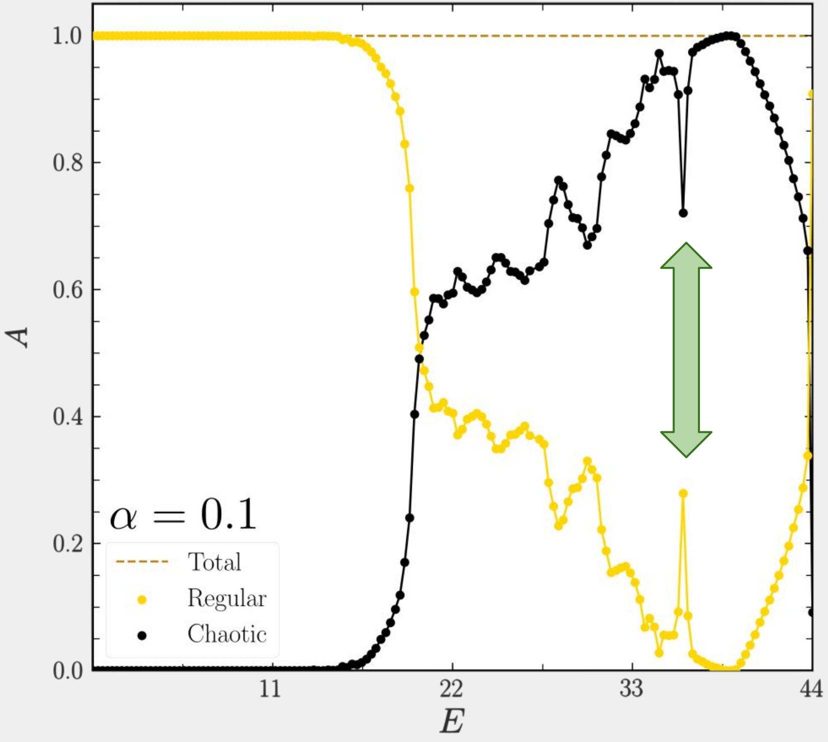
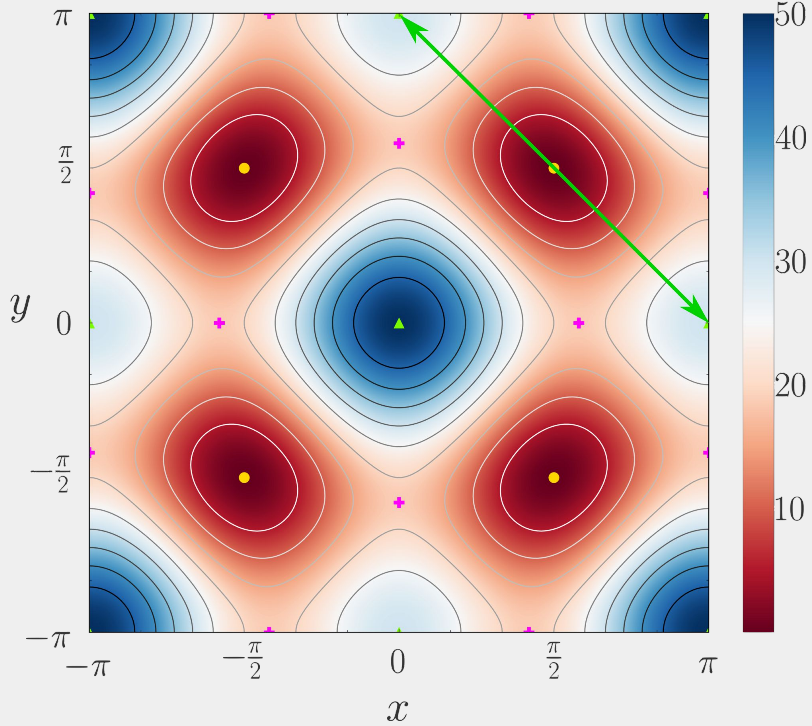
SALI results

- Area measurement by SALI

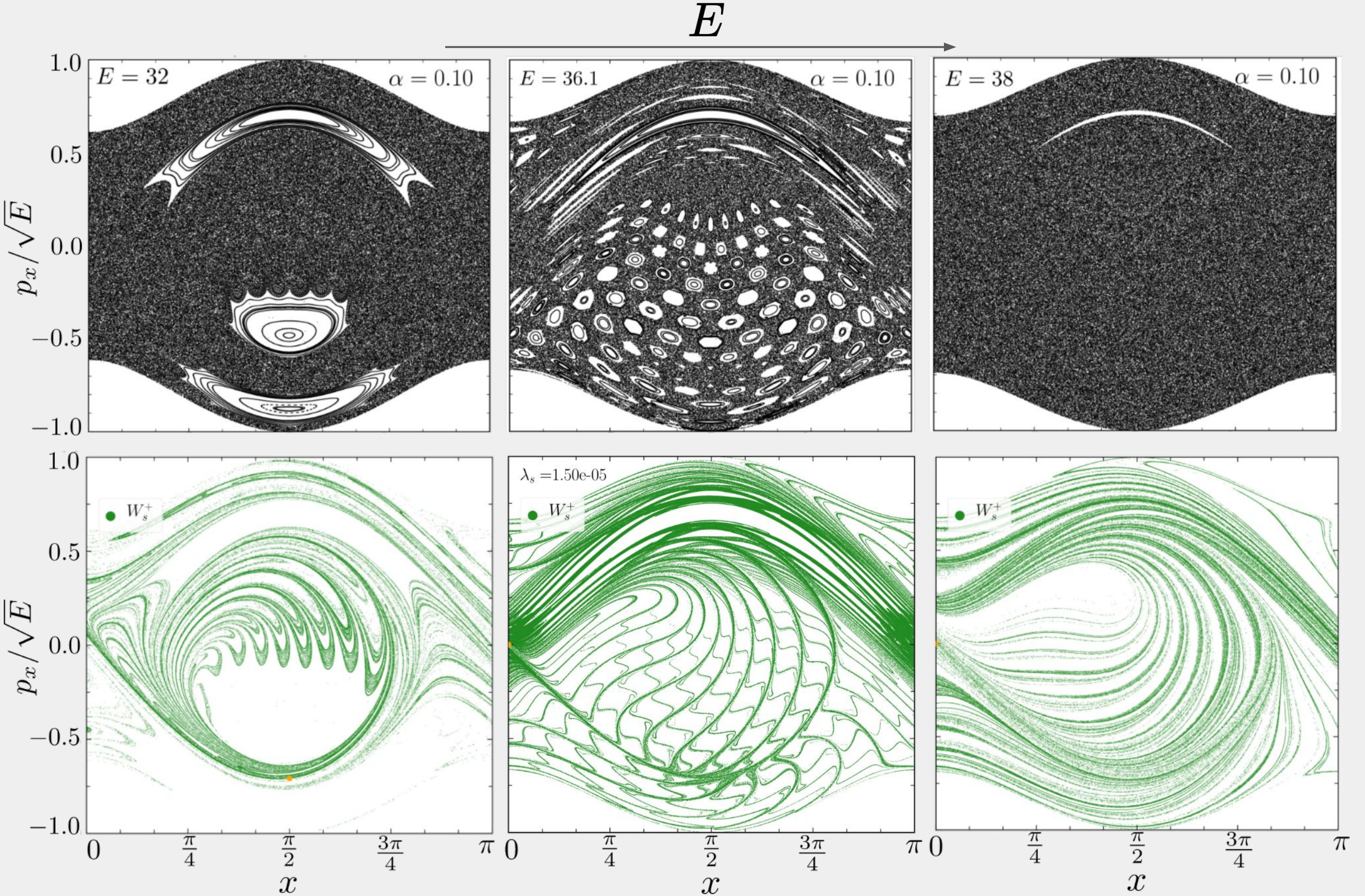


- At the energy level of **local maxima**, particles can reach unstable points



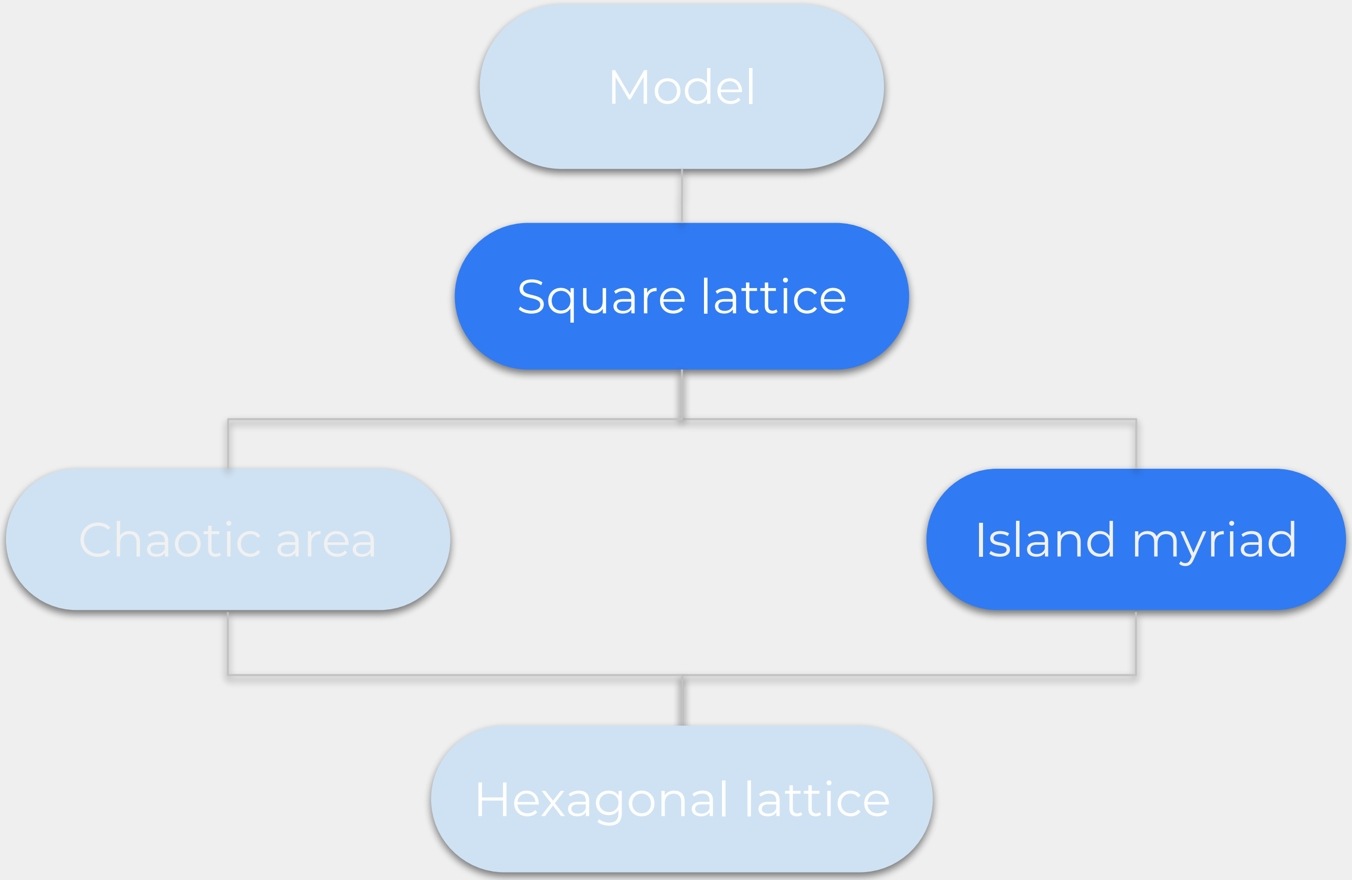
- Sudden **peak** (**drop**) in **stable** (**chaotic**) area at $E = 36.0$

Phase space



E
$E = 32$
$\alpha = 0.10$
$E = 36.1$
$\alpha = 0.10$
$E = 38$
$\alpha = 0.10$
$p_x/\sqrt{E}$
1.0
0.5
0.0
−0.5
−1.0
λ_s =1.50e-05
W_s^+
W_s^+
W_s^+
0
$\frac{\pi}{4}$
$\frac{\pi}{2}$
$\frac{3\pi}{4}$
π
x

Summary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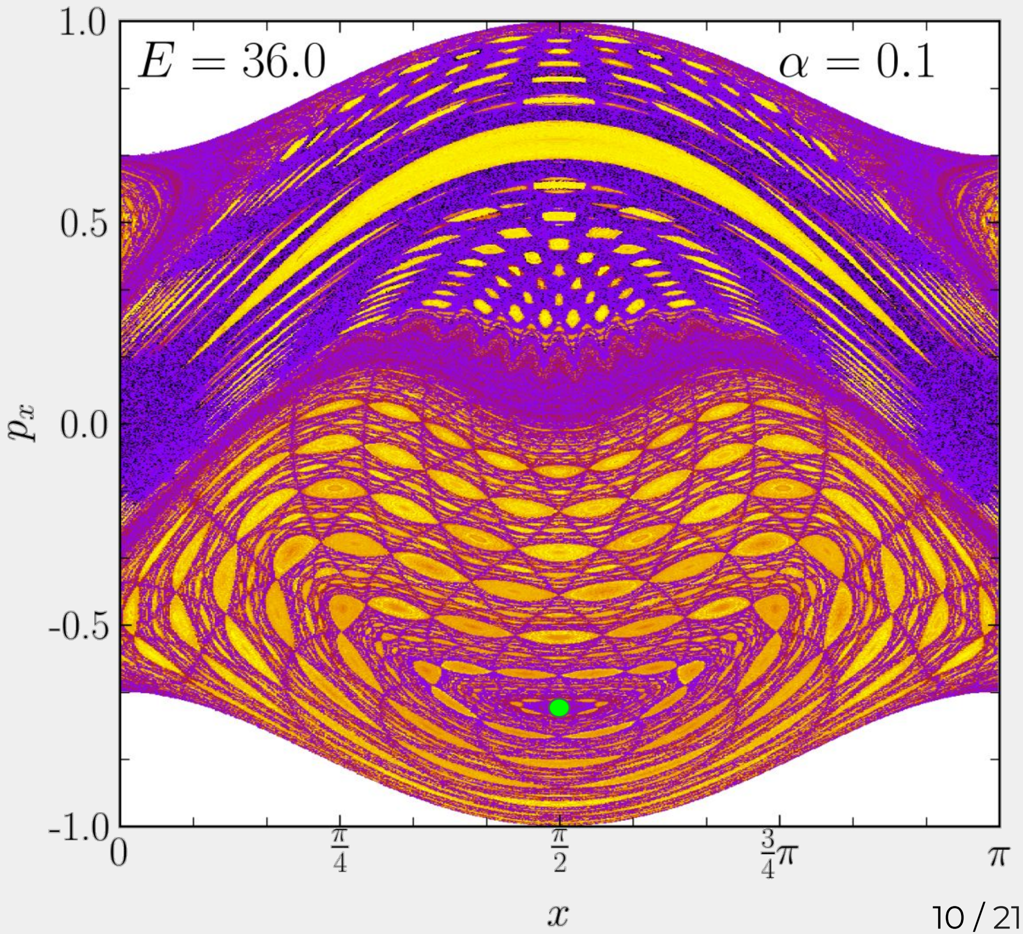
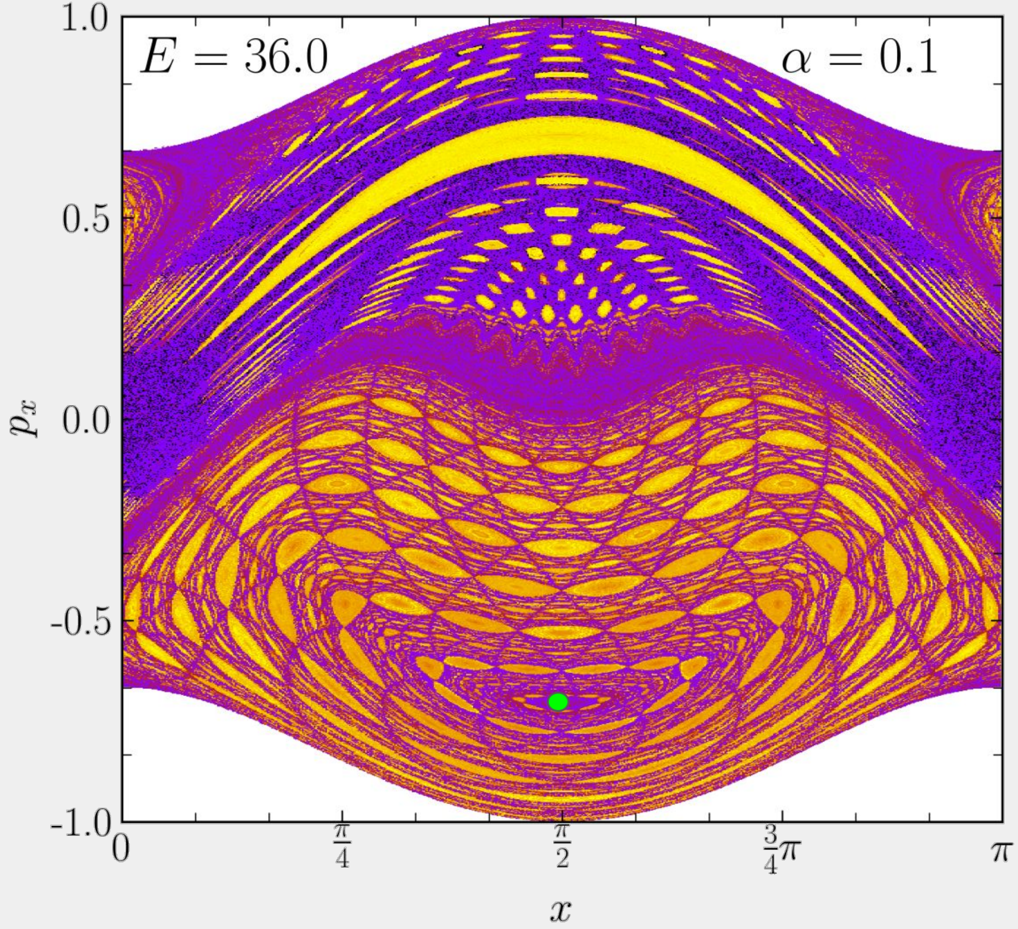
Island myriad bifurcation

- Set of island chains in an onion-like structure
  - Even periodicity
  - **Centered around** the unstable UPO over local maxima points
  - Isochronous chains (independent periodic orbits)
- Prominent fractal structure.
- Existence for short energy interval ($\Delta E \approx 0.5$).



Fractality



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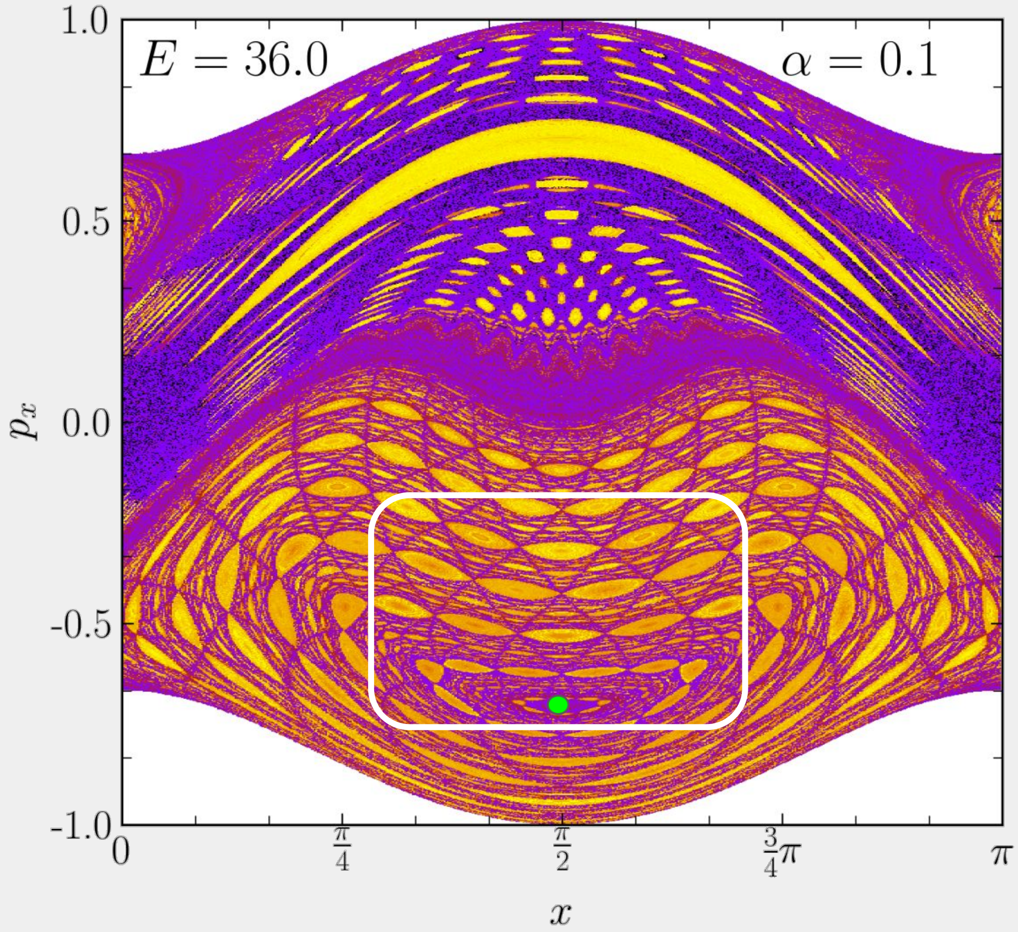

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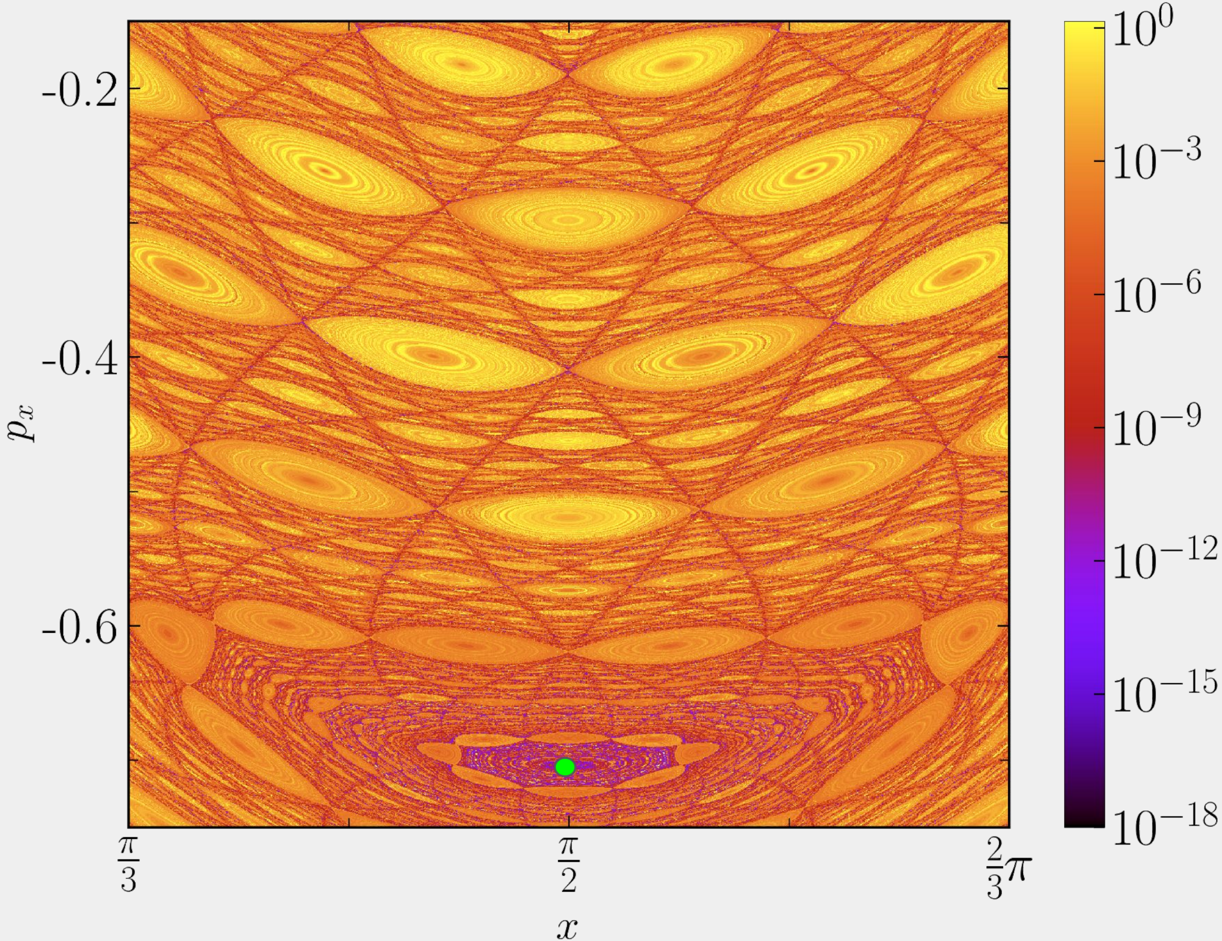
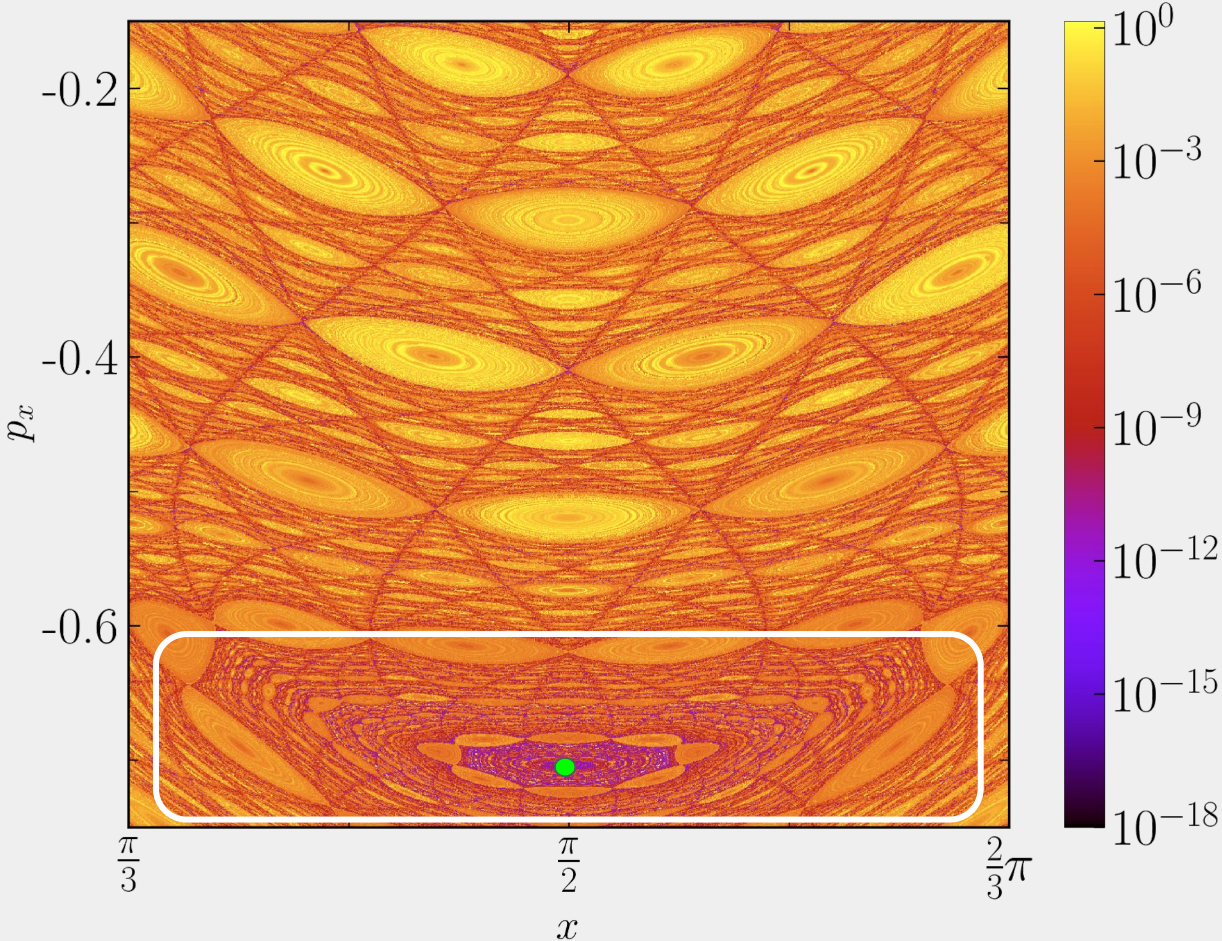


-0.2
-0.4
-0.6
p_x
$\frac{\pi}{3}$
$\frac{\pi}{2}$
$\frac{2}{3}\pi$
x
10^{0}
10^{-3}
10^{-6}
10^{-9}
10^{-12}
10^{-15}
10^{-18}

Fractality



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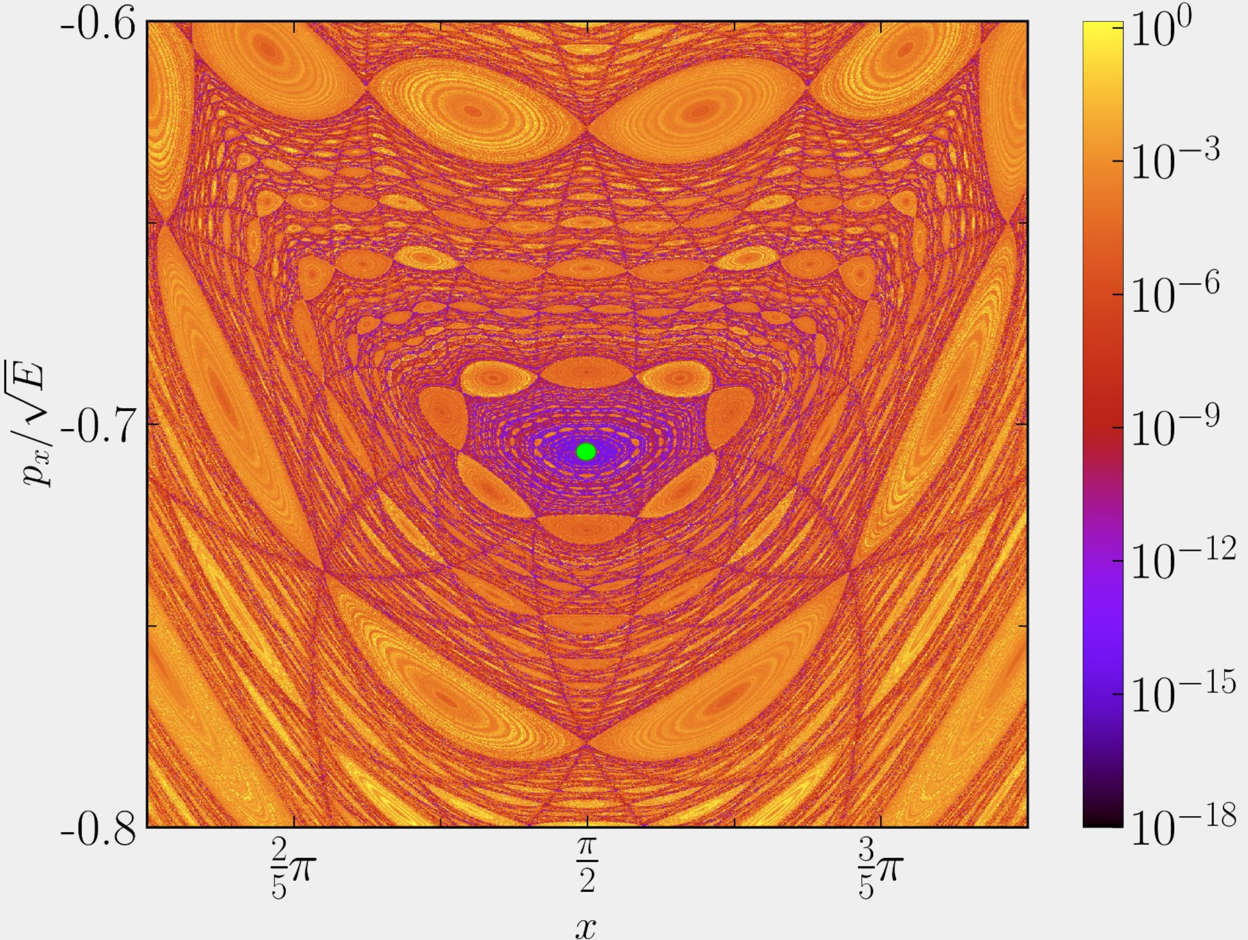
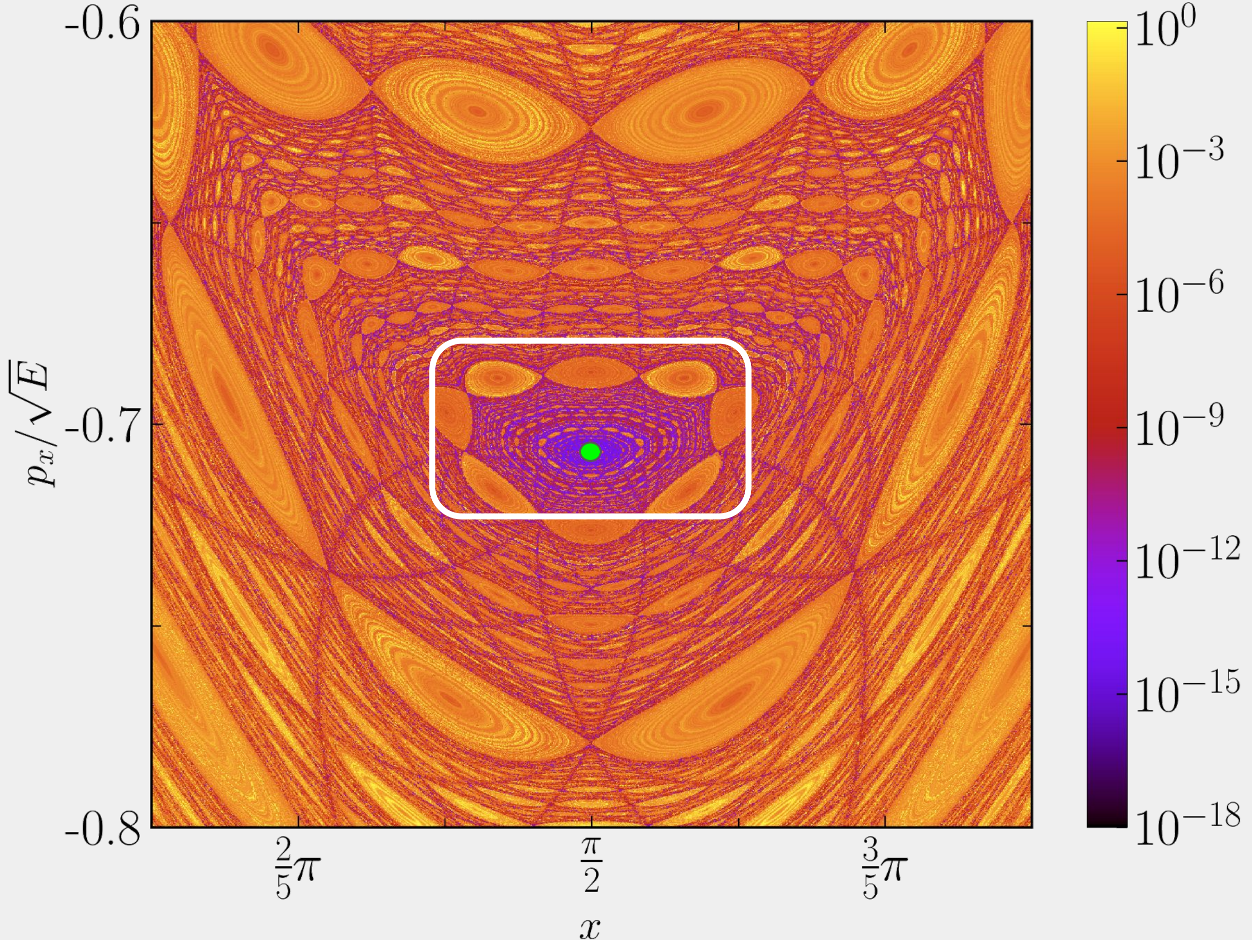


-0.6
-0.7
-0.8
$p_x/\sqrt{E}$
$\frac{2}{5}\pi$
$\frac{\pi}{2}$
$\frac{3}{5}\pi$
x
10^{0}
10^{-3}
10^{-6}
10^{-9}
10^{-12}
10^{-15}
10^{-18}

Fractality



-0.6
-0.7
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$p_x/\sqrt{E}$
$\frac{2}{5}\pi$
$\frac{\pi}{2}$
$\frac{3}{5}\pi$
x
10^0
10^{-3}
10^{-6}
10^{-9}
10^{-12}
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10^{-18}

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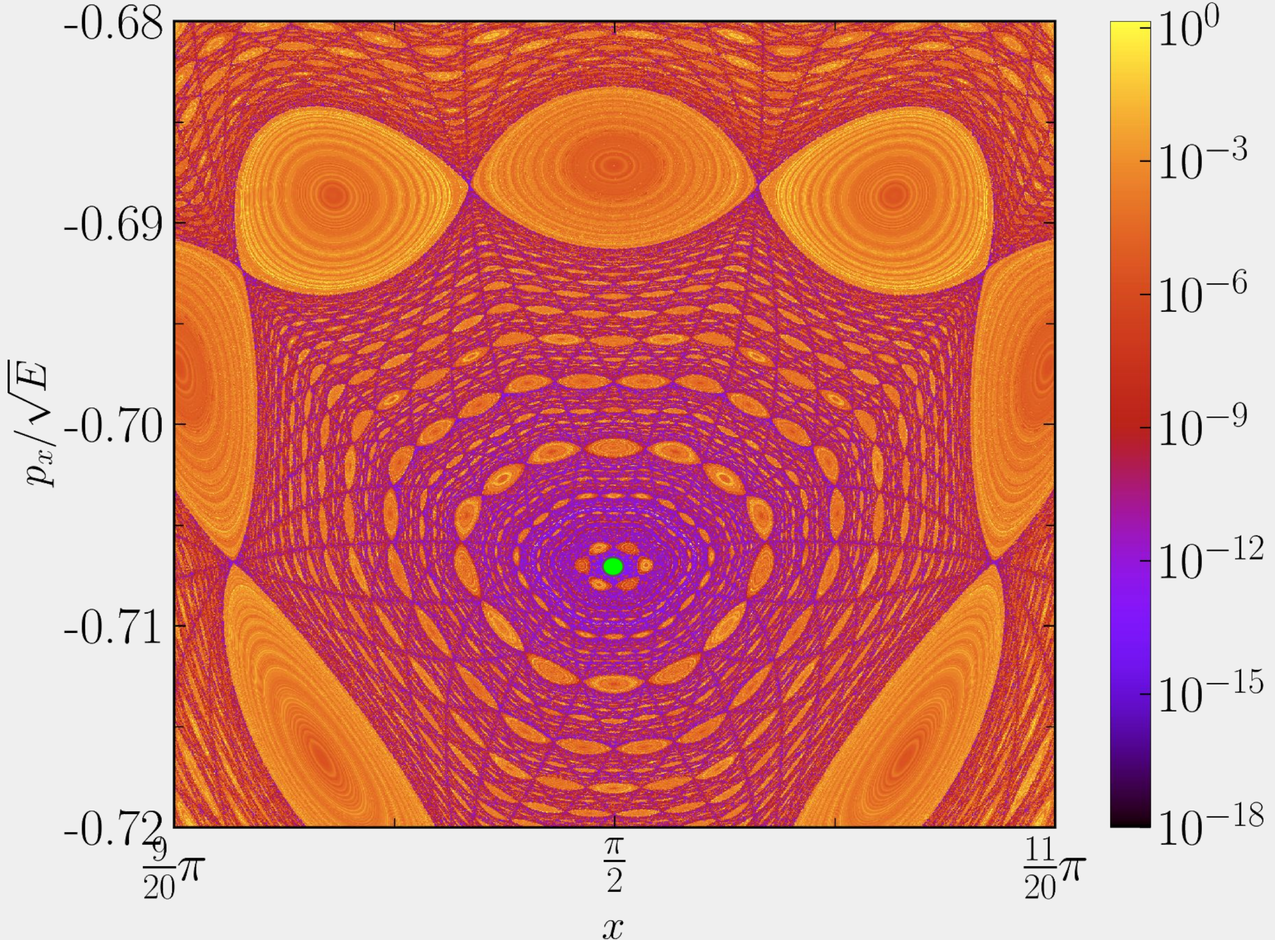

-0.68
-0.69
-0.70
-0.71
-0.72
$p_x/\sqrt{E}$
$\frac{9}{20}\pi$
$\frac{\pi}{2}$
$\frac{11}{20}\pi$
x
10^{0}
10^{-3}
10^{-6}
10^{-9}
10^{-12}
10^{-15}
10^{-18}

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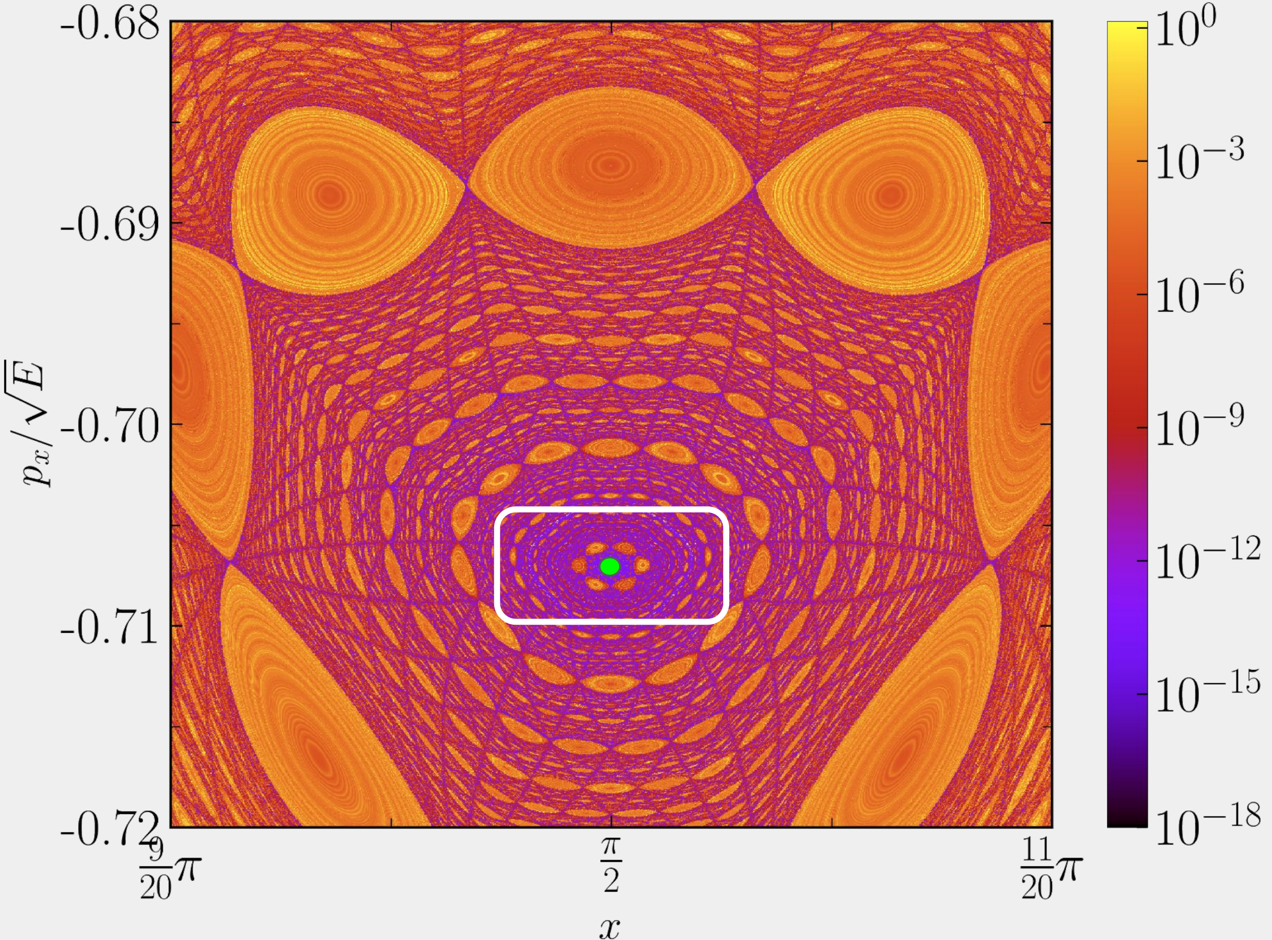

-0.68
-0.69
-0.70
-0.71
-0.72
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10^{0}
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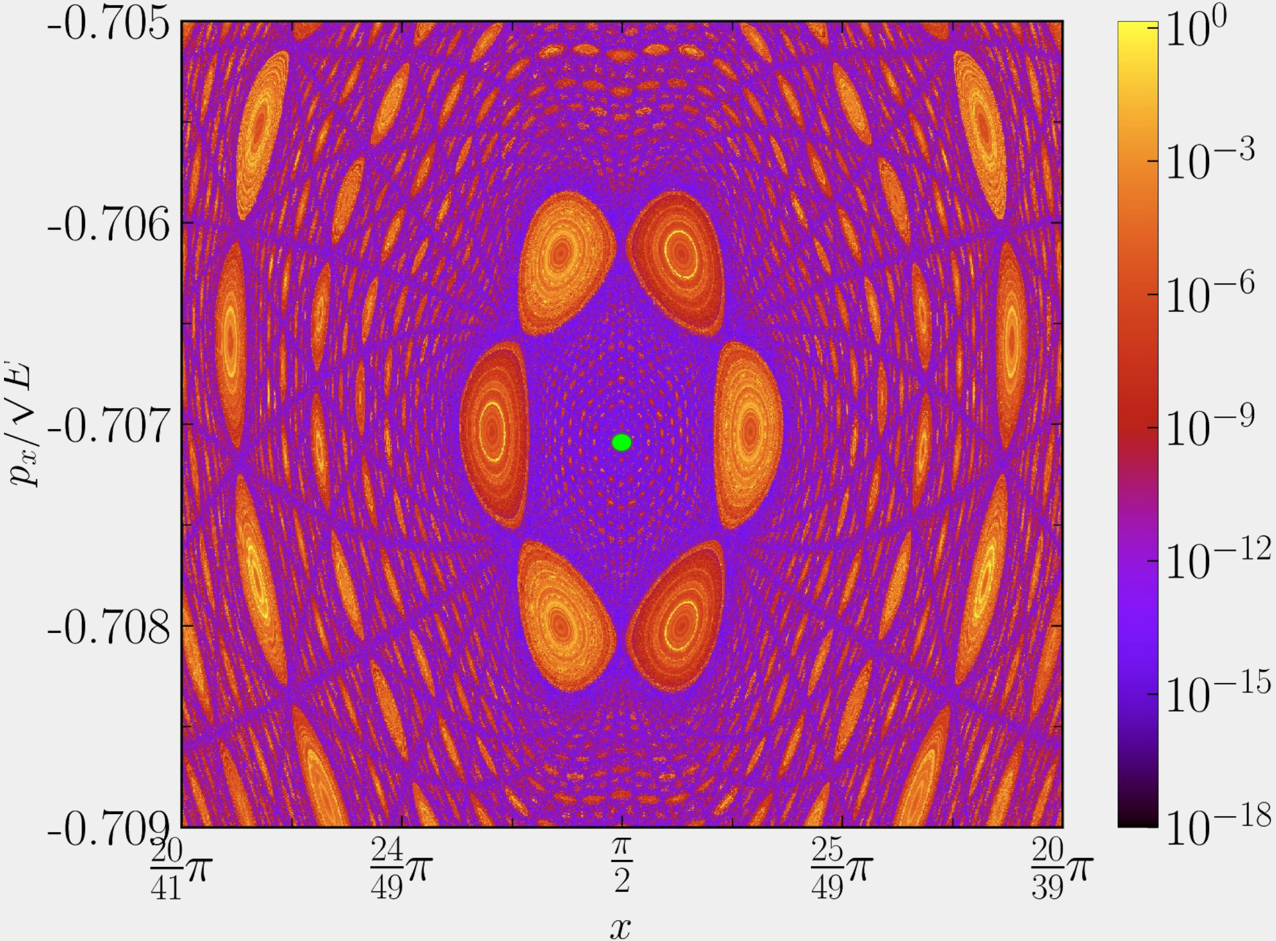
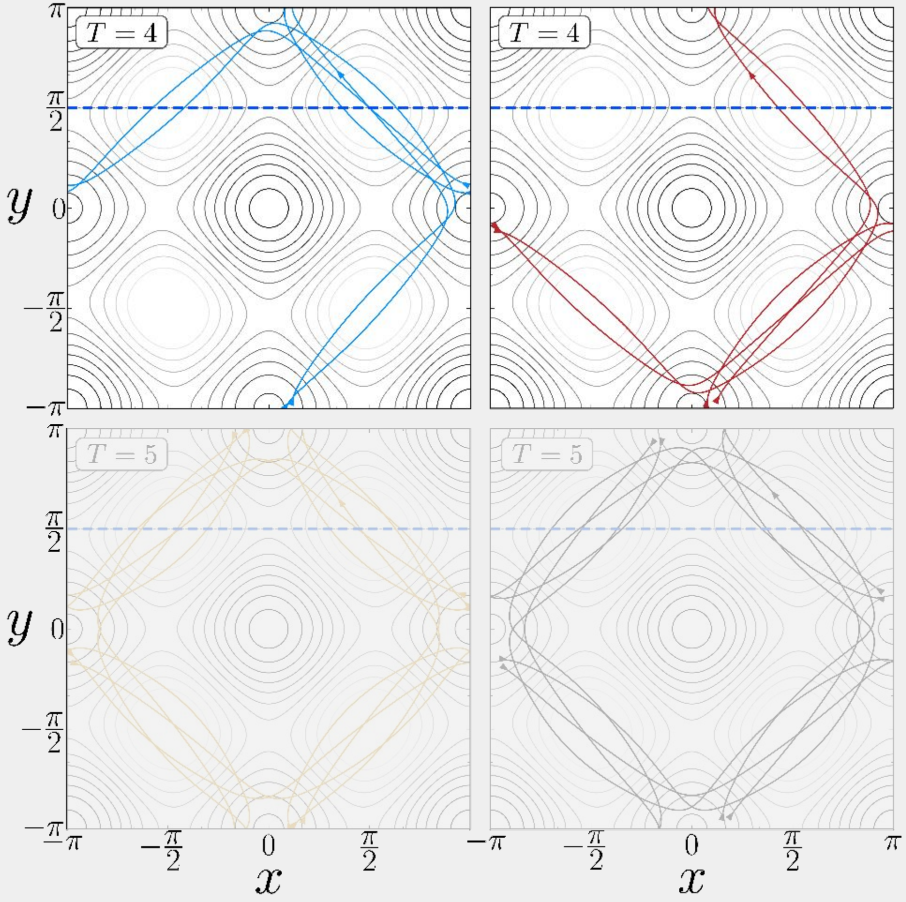
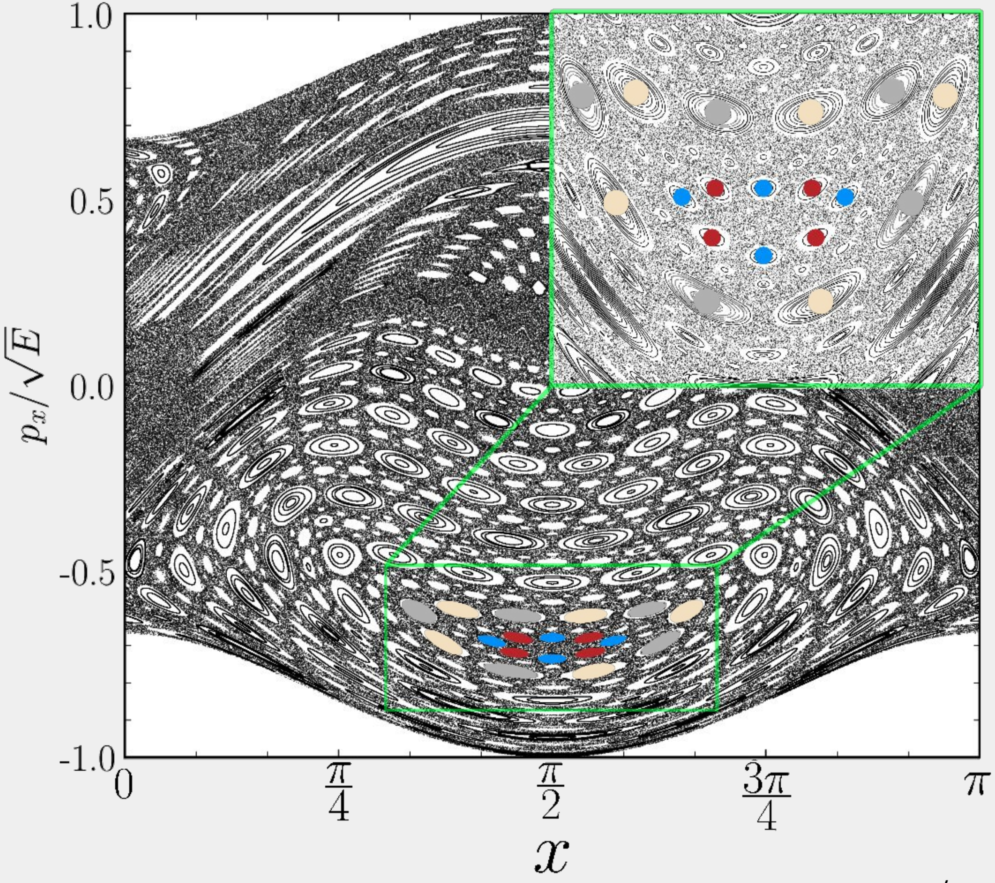


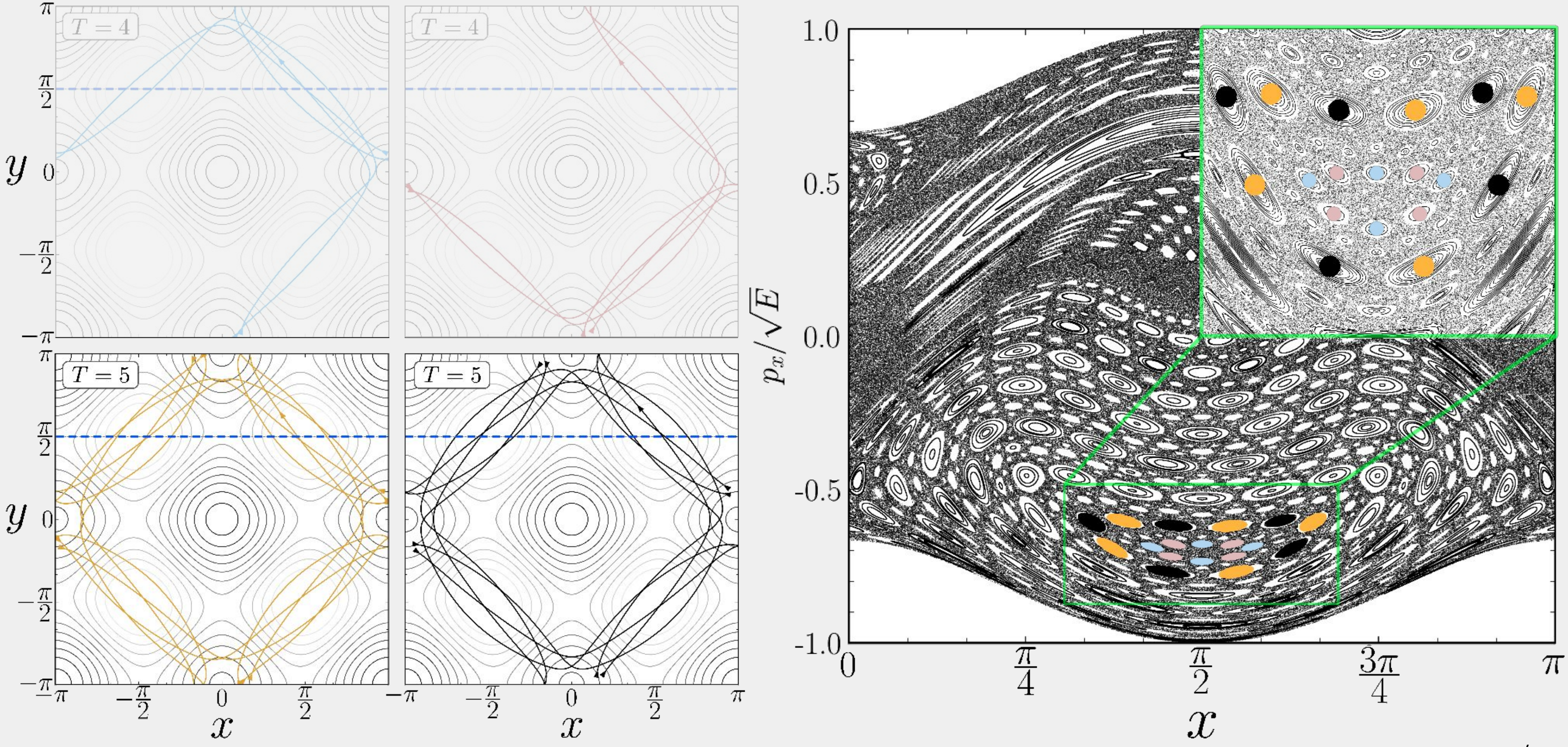
-0.705
-0.706
-0.707
-0.708
-0.709
$p_x/\sqrt{E}$
$\frac{20}{41}\pi$
$\frac{24}{49}\pi$
$\frac{\pi}{2}$
$\frac{25}{49}\pi$
$\frac{20}{39}\pi$
x
10^0
10^{-3}
10^{-6}
10^{-9}
10^{-12}
10^{-15}
10^{-18}

Isochronous chains



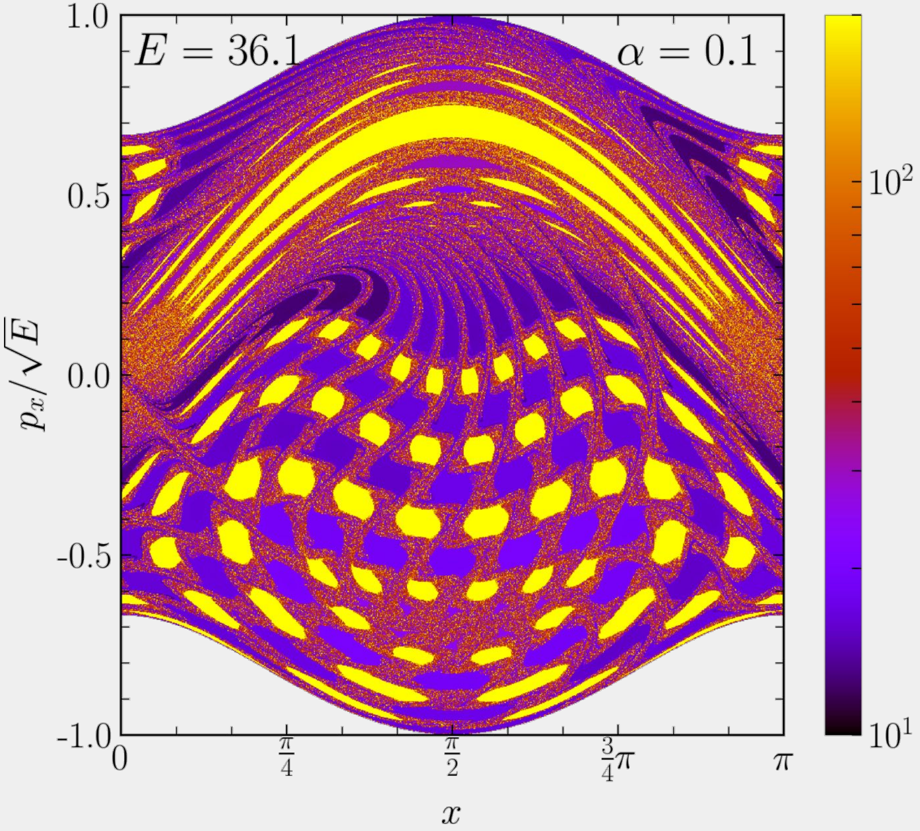


Isochronous chains



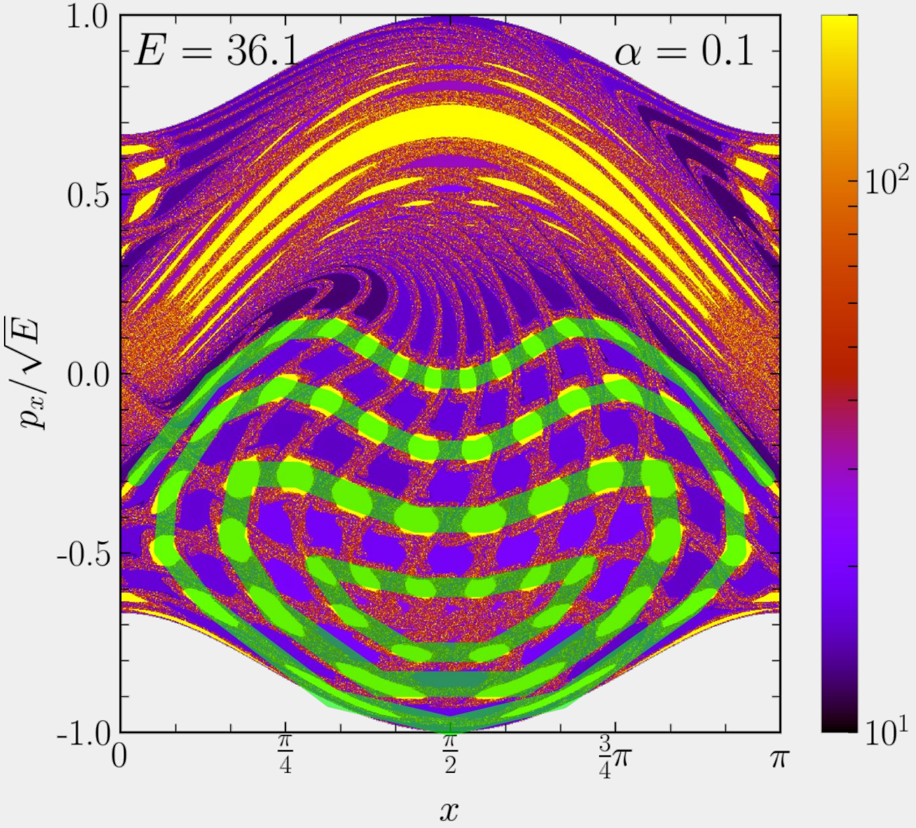
Escape time

- Alternating layers with either **trapped orbits** or **quick escape** through the lattice.

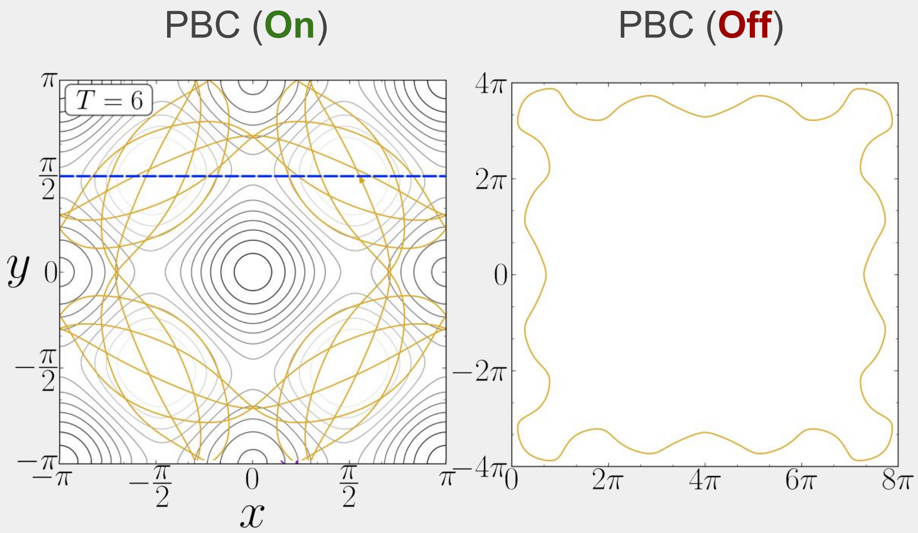


Escape time – spatially closed orbits

- Trapped orbits present spatial closure — return to its initial position without PBC



Libration (**closed orbit**)

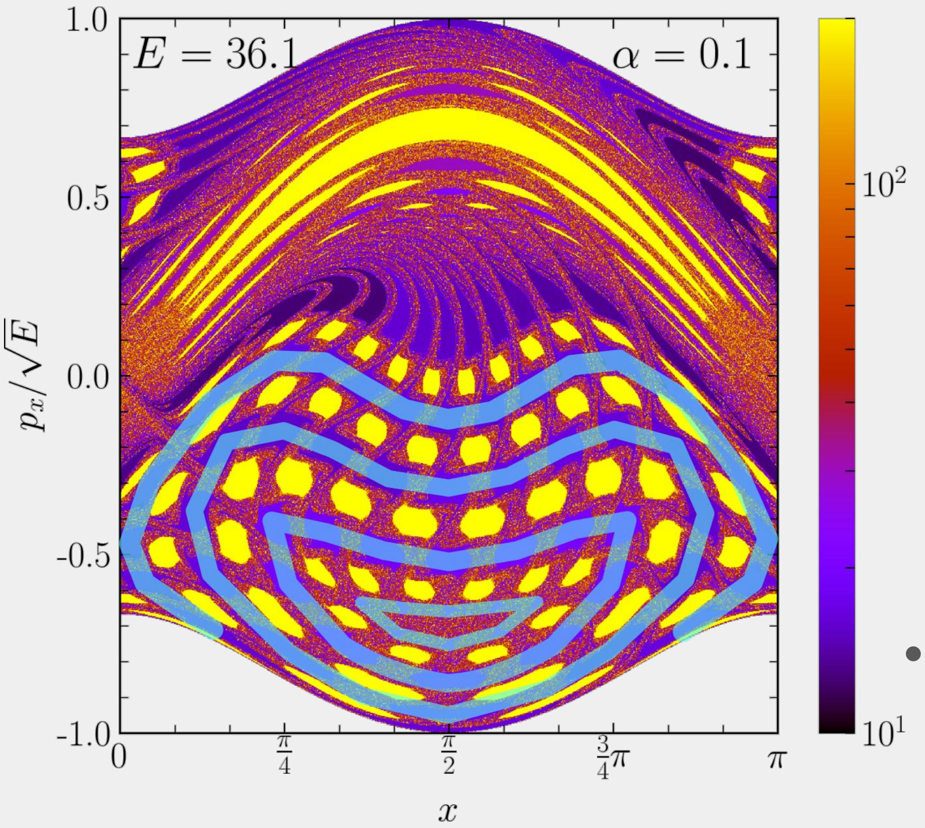


- Periodic return to original state

$$(x(t), y(t)) = (x(t+\tau), y(t+\tau)) \iff x, y \in \mathbb{R}$$

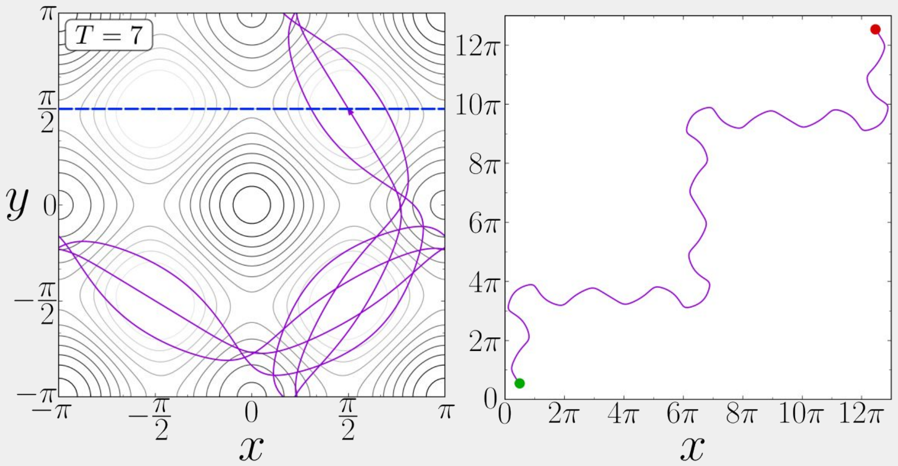
Escape time – spatially open orbits

- Direct flights lack spatial closure — return to initial position only when considering PBC



Rotation (**open orbit**)

PBC (**On**) PBC (**Off**)



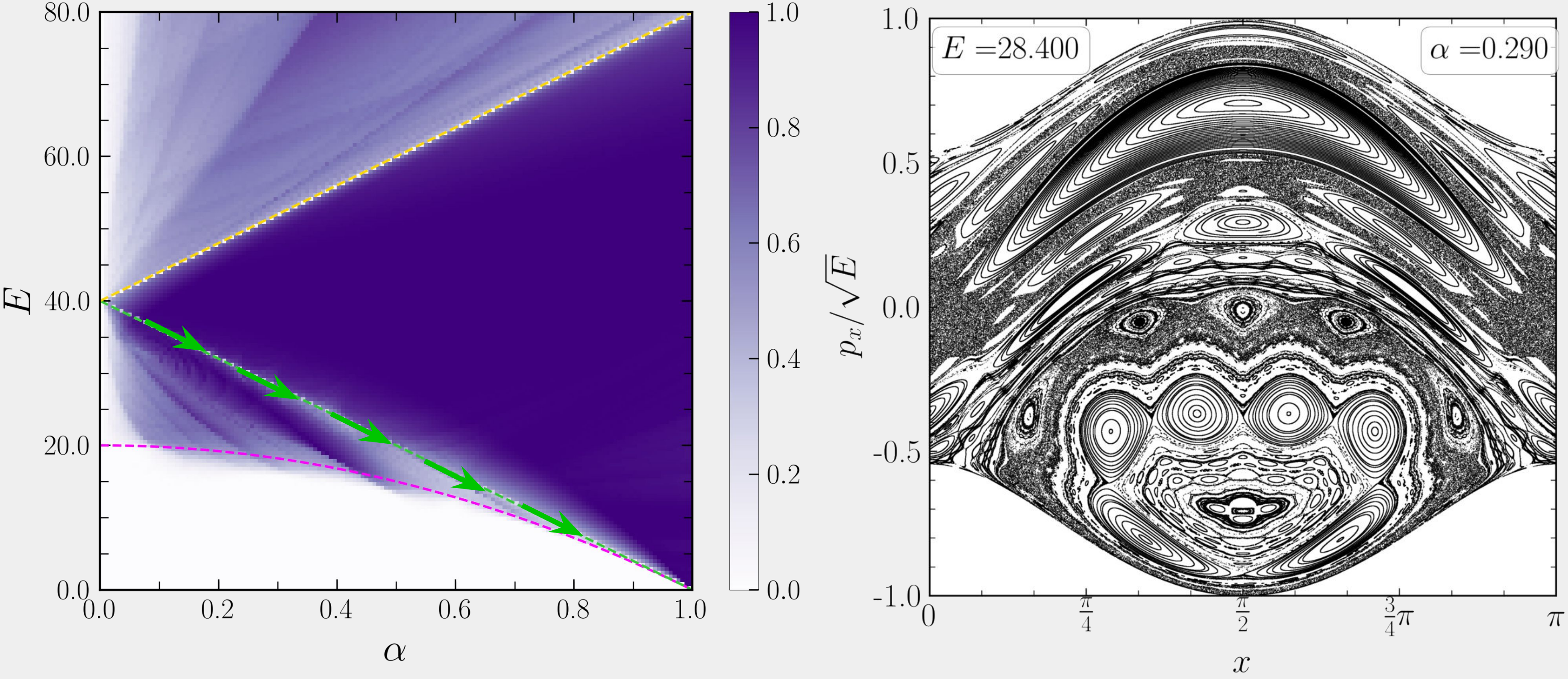
- Periodic return to an identical site in neighbor cell

$$(x(t), y(t)) = (x(t+\tau), y(t+\tau))$$

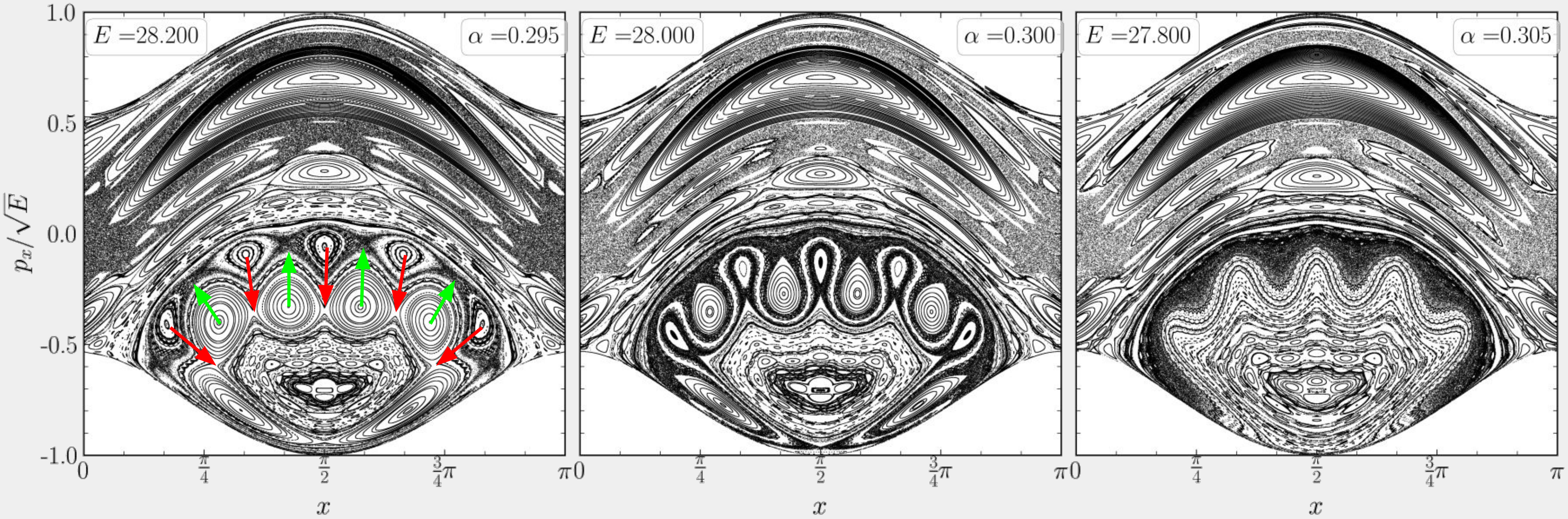
$$\Updownarrow$$

$$(x, y) \in (-\pi, \pi] \times (-\pi, \pi]$$

Separatrix reconnection



Separatrix reconnection

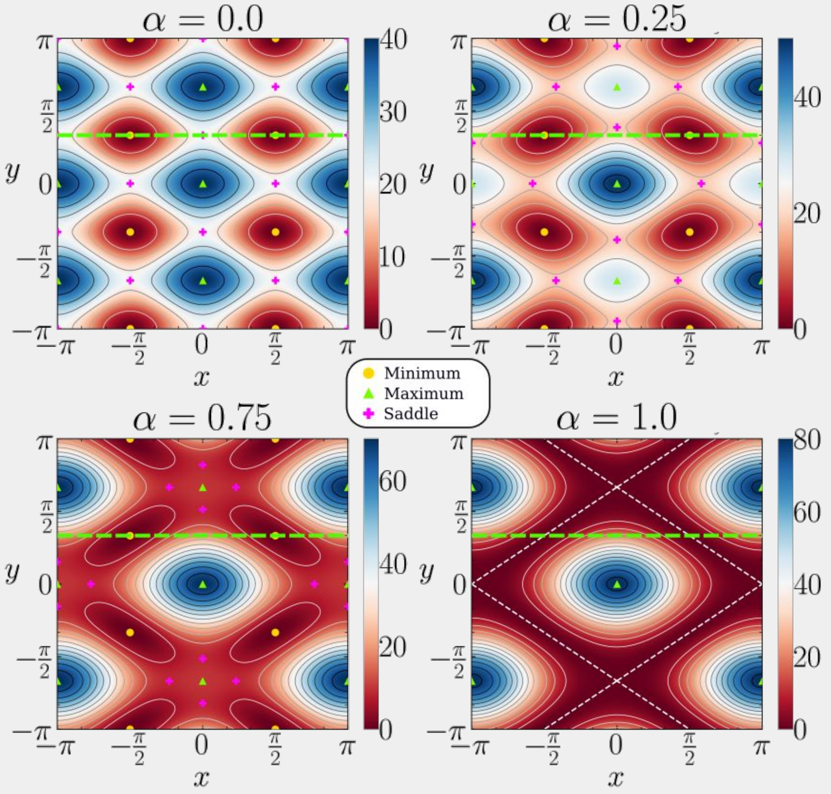


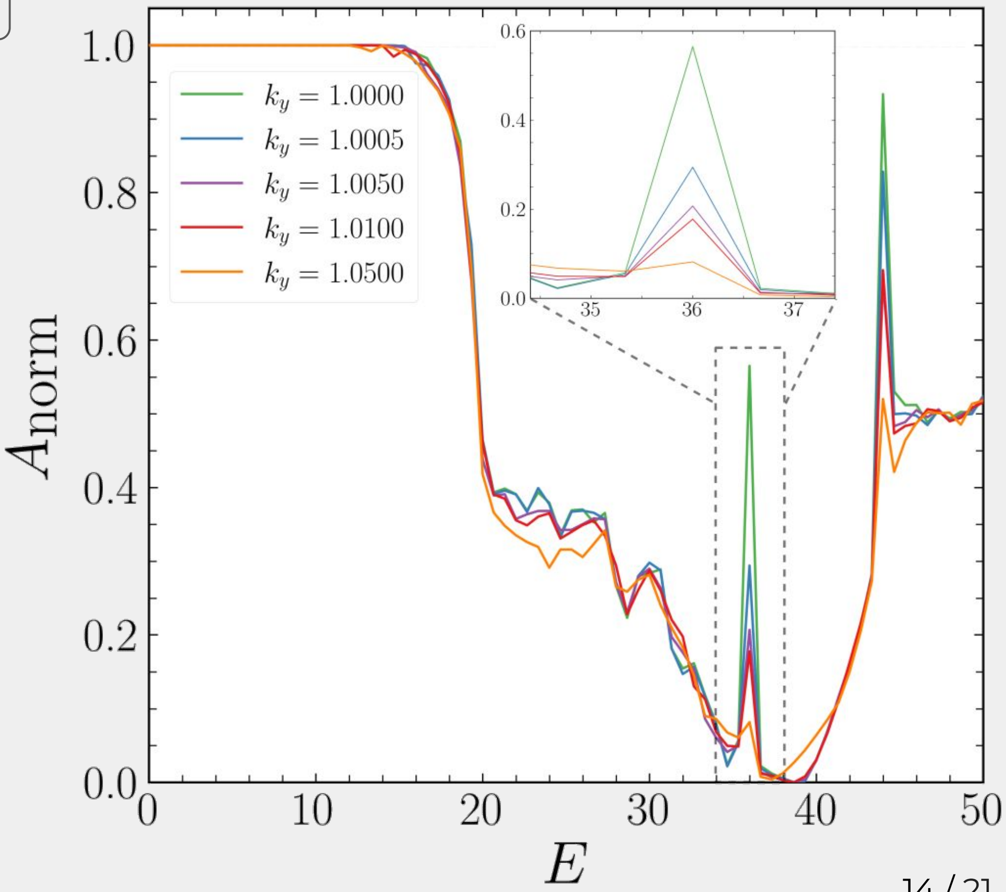
- Topological inversion between **outer** and **inner** island chains (separatrix reconnection)
- Myriad ‘peeling’ – repeated collision of islands as inner chains move outwards
- Local **non-twist** winding number profile

How resilient is the myriad structure under symmetry break...?

Symmetry break – Rectangular lattice

$$V(x,y) = U\left(\cos^2(x) + \cos^2(k_y y) + 2\alpha\cos(x)\cos(k_y y)\right)$$





Periodic orbits calculation - Monodromy method

Near a periodic orbit, displacements are linearly described by the **monodromy matrix**[1]:

$$\delta\vec{s}(\tau) = \mathbf{M}\,\delta\vec{s}(0)$$

Numerically, displacements $\delta\vec{s}_i = (\delta x^i, \delta y^i, \delta p_x^i, \delta p_y^i)$ around a near periodic orbit $\vec{s} = \{\vec{s}_1, ..., \vec{s}_N\}$, where $\vec{s}_i = \{x^i, y^i, p_x^i, p_y^i\}$, are

$$\delta\vec{s}_{N+1} = \mathbf{\Lambda}_{N+1}\delta\vec{s}_1 + \mathbf{\Gamma}_{N+1}$$

Imposing the orbit's closure condition ($\delta\vec{s}_{N+1} = \delta\vec{s}_1$), returns a linear system for the first displacement correction:

$$\left(\mathbf{I}_4 - \mathbf{\Lambda}_{N+1}\right)\delta\vec{s}_1 = \mathbf{\Gamma}_{N+1}$$

The corrected orbit is iterated until convergence: $|\mathbf{\Gamma}_{N+1}| \to 0$ (Newton-Raphson)

[1] M. Baranger *et al.* Annals of Physics **186** (1988)

Periodic orbits calculation - Monodromy method

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Imposing the orbit's closure condition ($\delta\vec{s}_{N+1} = \delta\vec{s}_1$), returns a linear system for the first displacement correction[2]:

$$\left(\mathbf{I}_4 - \mathbf{\Lambda}_{N+1} + \frac{1}{\epsilon_0}\mathbf{\Delta}_{N+1} \otimes \Theta\right)\delta\vec{s}_1 = \mathbf{\Gamma}_{N+1} + \frac{\eta}{\epsilon_0}\mathbf{\Delta}_{N+1}$$

Besides Γ, the scalar η is now used for energy convergence.

[1] M. Baranger *et al.* Annals of Physics **186** (1988)

[2] N. S. Simonovic, Chaos **9(4)**, (1999)

Periodic orbits calculation - Monodromy method

As shown previously, the converged orbit will have the same period as the initial guess. For a PO with a given energy, the new linear system considers the time step (*i.e.* the period) as a new variable and the conservation of energy as extra equation[1]

$$\left(\mathbf{I}_4 - \mathbf{\Lambda}_{N+1} + \tfrac{1}{\epsilon_0}\mathbf{\Delta}_{N+1} \otimes \Theta\right) \delta\vec{s}_1 = \mathbf{\Gamma}_{N+1} + \tfrac{\eta}{\epsilon_0}\mathbf{\Delta}_{N+1}$$

Besides Γ, the scalar η is now used for energy convergence.

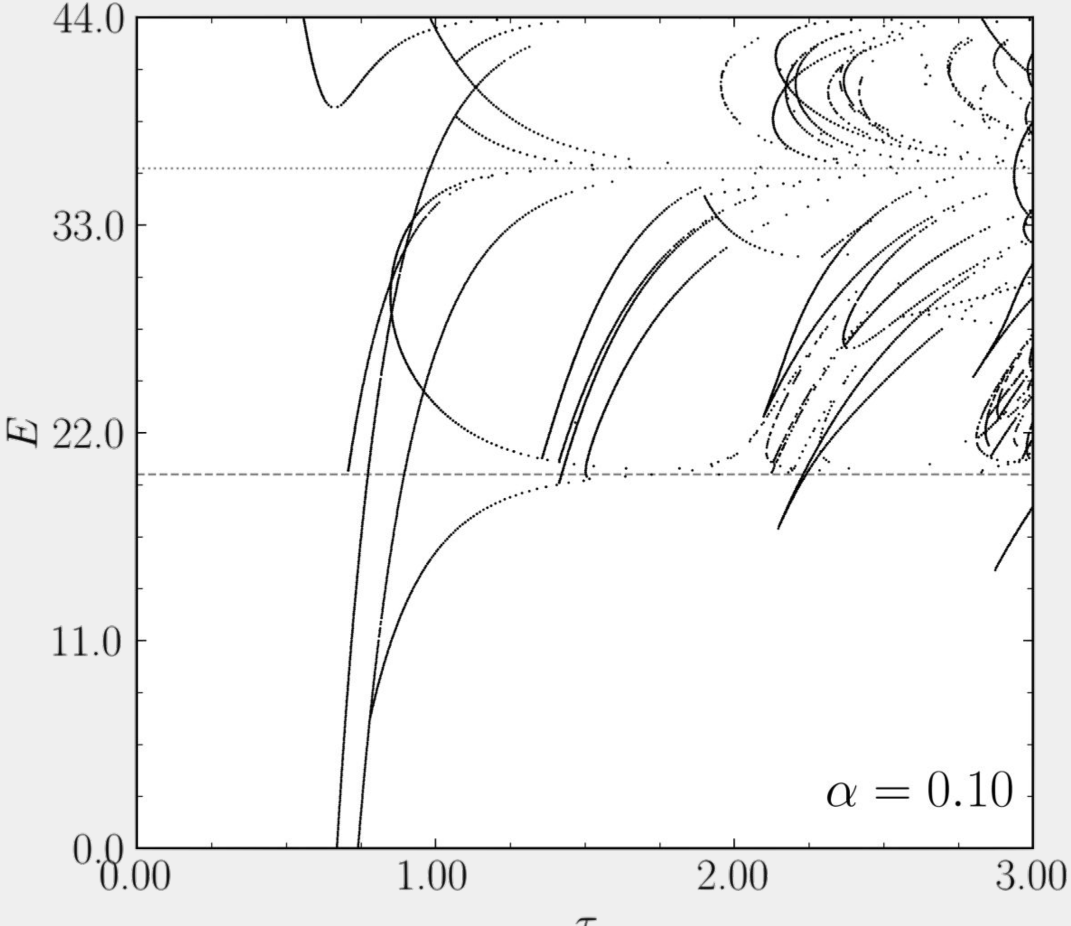
- The converged matrix $\mathbf{\Lambda}_{N+1}$ becomes the monodromy $\mathbf{M}$
- For 2D systems, $\mathbf{M}$ immediately provides the orbit stability from its trace:

$$\text{stable} \longrightarrow \text{tr}(\mathbf{M}) = 2 \pm (e^{i\theta\tau} + e^{-i\theta\tau}) = 2(1 \pm \cos(\theta\tau)) \in [0, 4]$$

$$\text{unstable} \longrightarrow \text{tr}(\mathbf{M}) = 2 \pm (e^{\theta\tau} + e^{-\theta\tau}) = 2(1 \pm \cosh(\theta\tau)) \in (-\infty, 0] \cup [4, \infty)$$

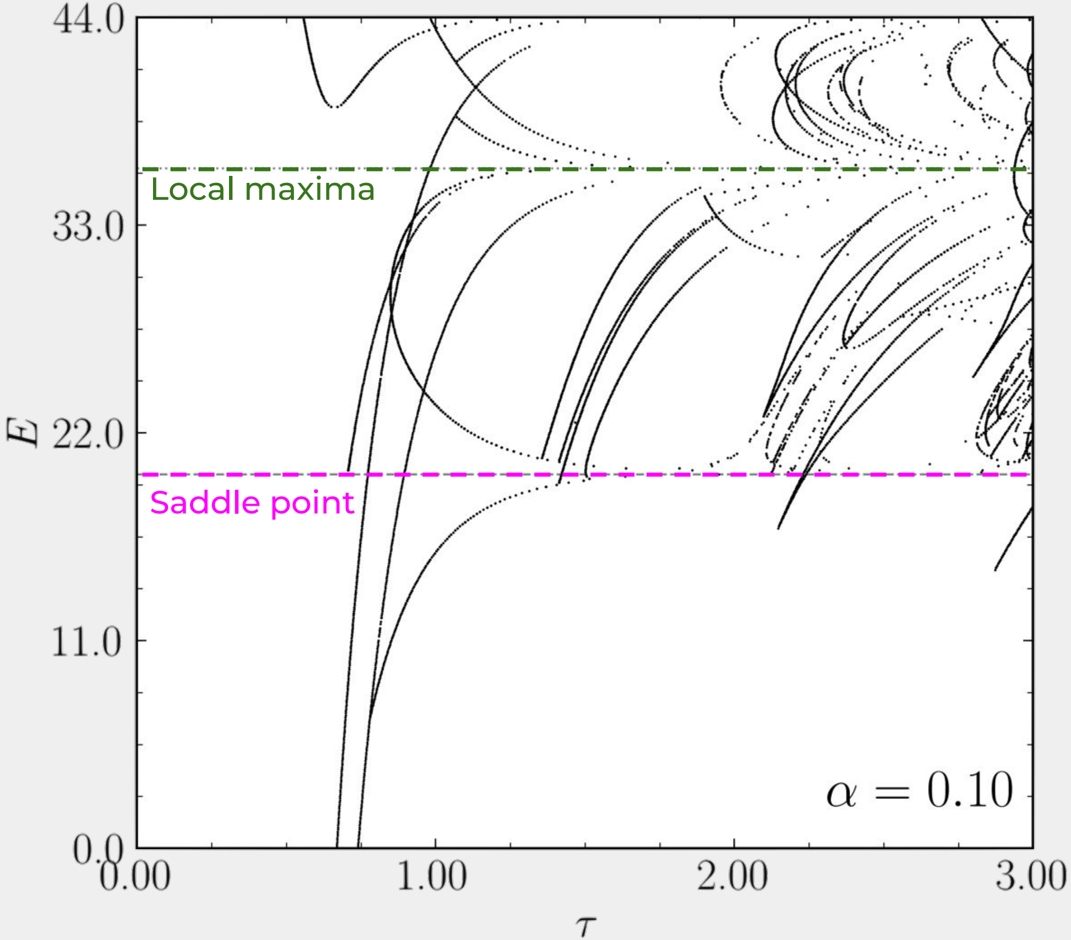
[1] N. S. Simonovic, Chaos **9(4)**, (1999)

Periodic orbits - Energy x Period diagram



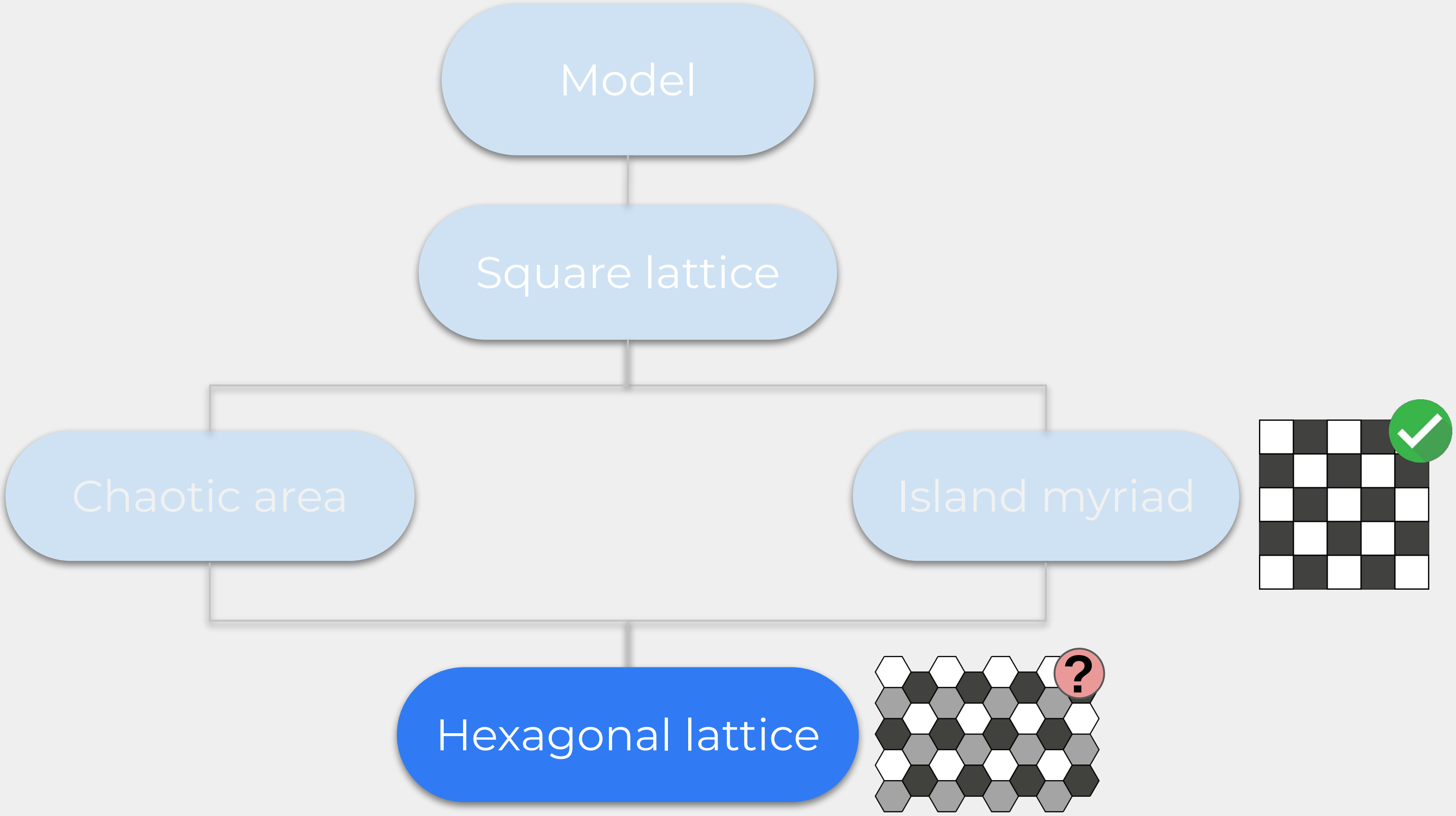
- Periodic orbits search over phase space (for fixed parameters) – map period **1** to **4**.

Periodic orbits - Energy x Period diagram



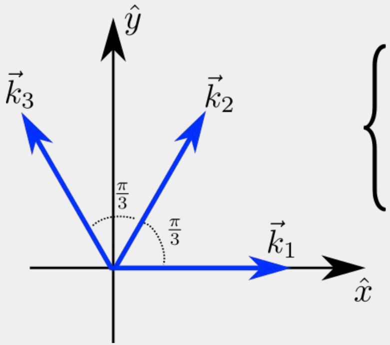
- Periodic orbits search over phase space (for fixed parameters) – map period **1** to **4**.
- Horizontal lines mark the energy level for saddle equilibria (E=19.8) and local maxima (E=36).
- A periodic orbit approaching an unstable equilibrium point diverges in period (classic pendulum analog).

Summary


Model
Square lattice
Chaotic area
Island myriad
Hexagonal lattice
?

Hamiltonian model - Hexagonal Lattice

- Investigation of the myriad phenomenon for a hexagonal lattice
- Lattice setup with three co-planar waves



$$\begin{cases} \vec{k}_1 = k\hat{x} \\ \vec{k}_2 = \frac{k}{2}\left(\hat{x} + \sqrt{3}\hat{y}\right) \\ \vec{k}_3 = \frac{k}{2}\left(-\hat{x} + \sqrt{3}\hat{y}\right) \end{cases}$$

$$\begin{aligned} V(x,y) = U\Bigg(& \cos^2(kx) + \cos^2\left(\frac{k}{2}x + \frac{\sqrt{3}k}{2}y\right) + \cos^2\left(-\frac{k}{2}x + \frac{\sqrt{3}k}{2}y\right) \\ & + 2\alpha_{12}\cos(kx)\cos\left(\frac{k}{2}x + \frac{\sqrt{3}k}{2}y\right) \\ & + 2\alpha_{13}\cos(kx)\cos\left(-\frac{k}{2}x + \frac{\sqrt{3}k}{2}y\right) \\ & + 2\alpha_{23}\cos\left(\frac{k}{2}x + \frac{\sqrt{3}k}{2}y\right)\cos\left(-\frac{k}{2}x + \frac{\sqrt{3}k}{2}y\right)\Bigg) \end{aligned}$$

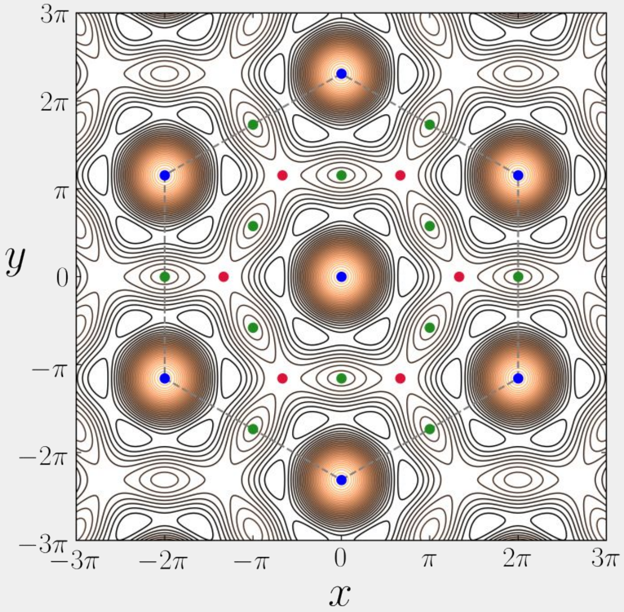
Single coupling condition

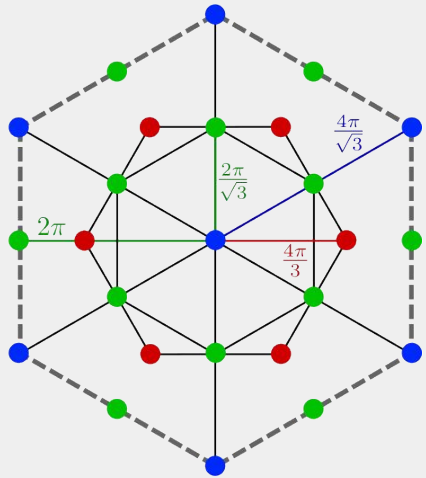
$$\alpha_{12} = \alpha_{13} = \alpha_{23} = \alpha$$

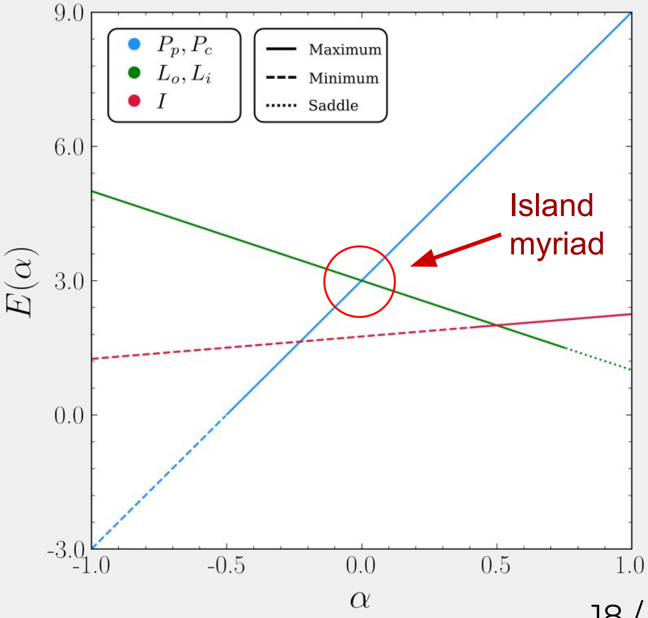
$$V(x,y,\alpha) = 1 + \cos\left(\sqrt{3}y\right)\left(\alpha + \cos(x)\right) + \cos(x)\left(4\alpha\cos\left(\frac{x}{2}\right)\cos\left(\frac{\sqrt{3}y}{2}\right) + \alpha + \cos(x)\right)$$

Honeycomb potential – Equilibrium points

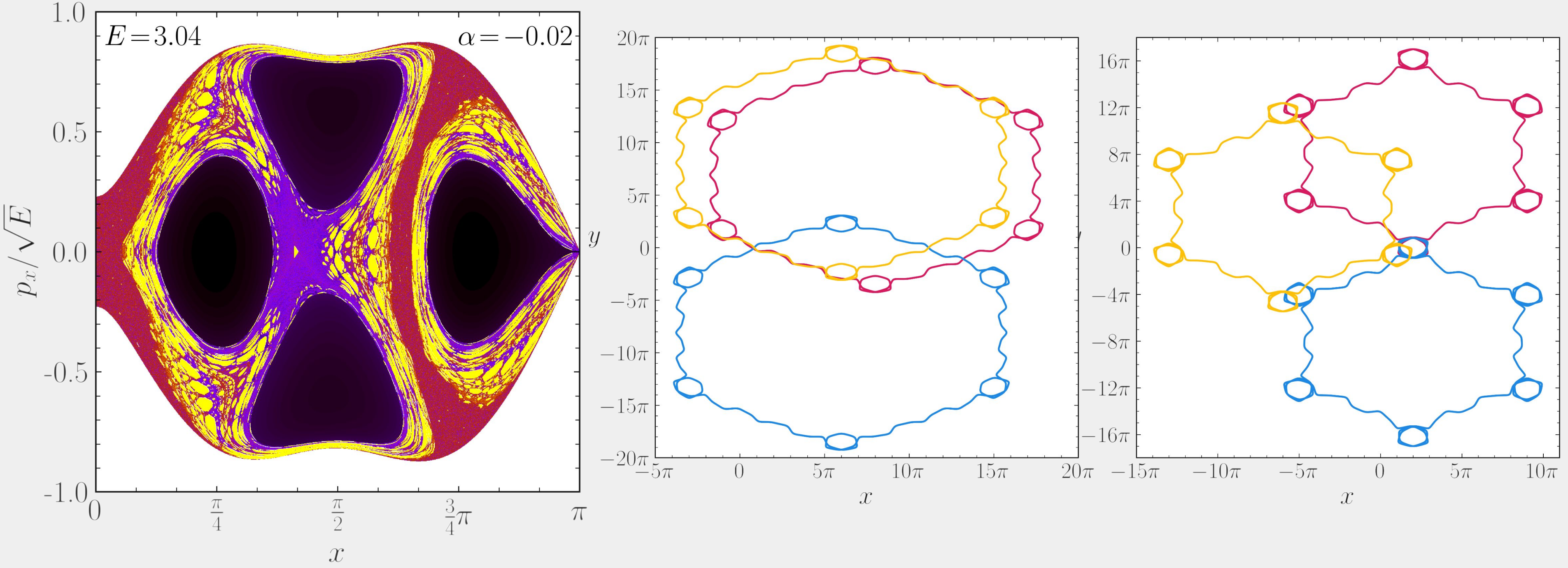
- Set of equilibrium points with fixed position as the coupling changes
- Conservation of hexagonal symmetry required by the myriad orbits
- Reference points for energy levels where the myriad is expected
- Island myriad found only near $\alpha \approx 0$







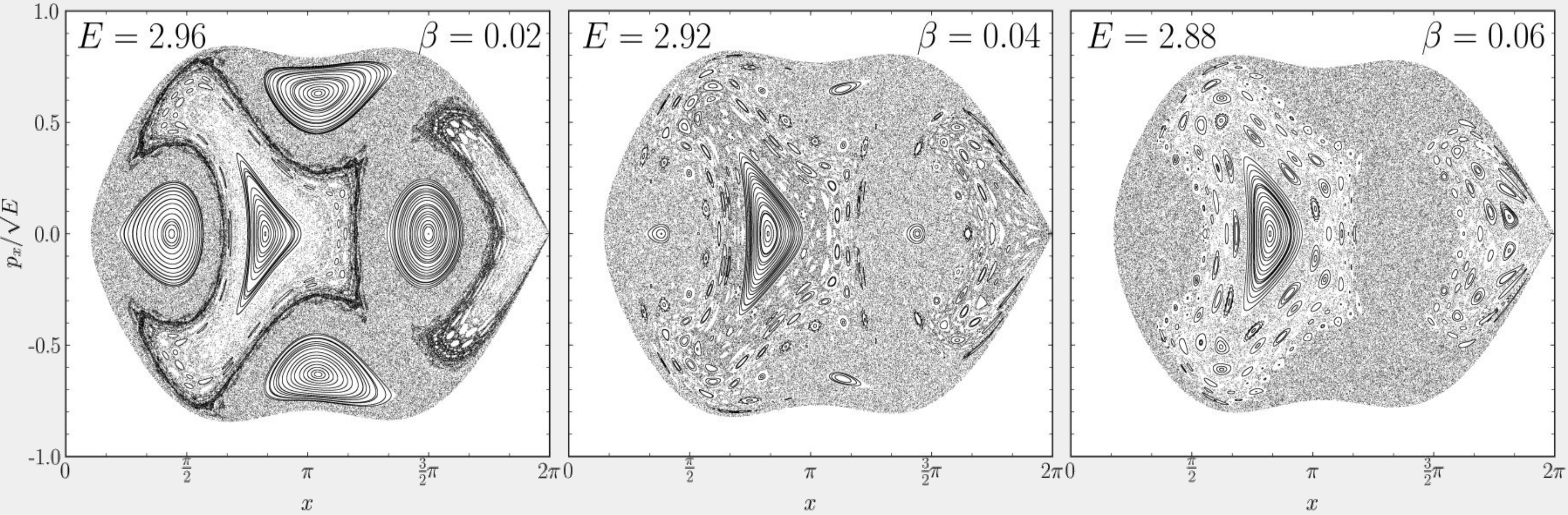
Honeycomb potential – island myriad ($\alpha \gtrsim 0$)



- Fractality is attenuated due to additional sources of instability within the potential surface
- Isochronous chains with triple multiplicity

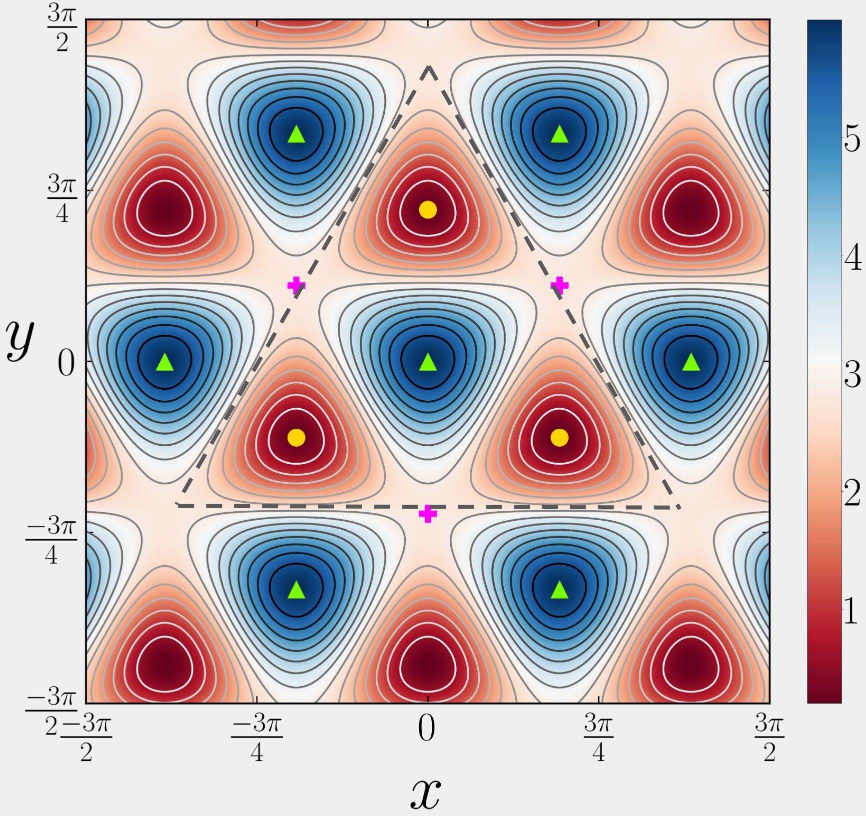
Honeycomb potential – Island myriad

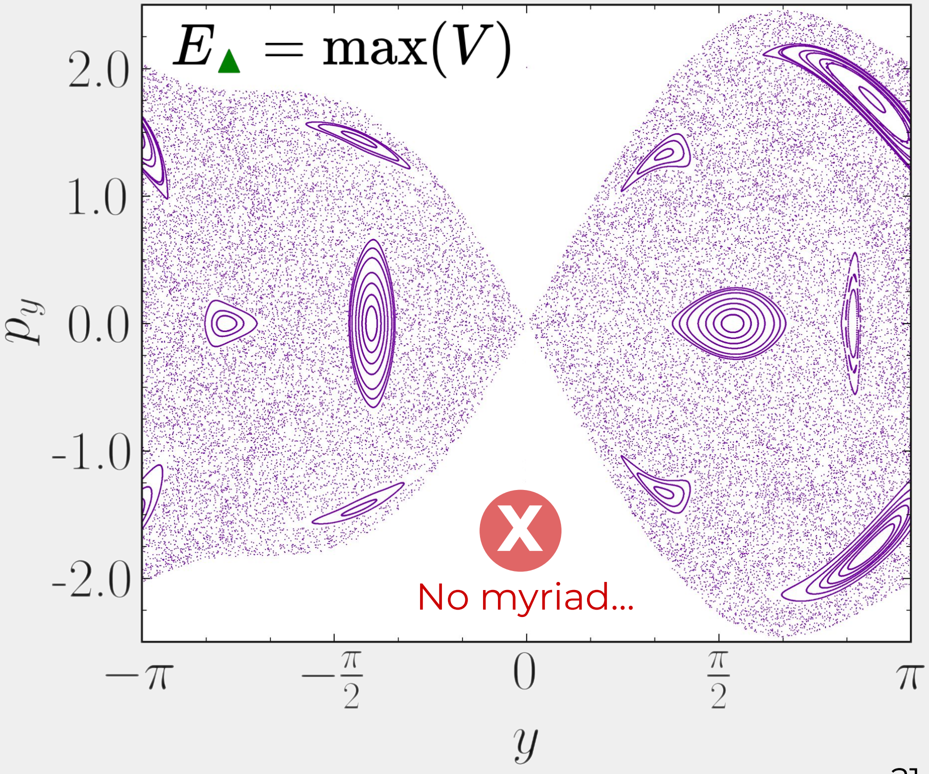
- Partial transport barrier from strong **stickiness**
- Existence of the myriad for a short coupling interval



Triangular lattice – Equilibrium points

$$V = 3 + \cos(\sqrt{3}x - y) + \frac{1}{2}\sin(\sqrt{3}x - y) + \left(2\cos\left(\frac{\sqrt{3}x}{2} - \frac{y}{2}\right) - \sin\left(\frac{\sqrt{3}x}{2} - \frac{y}{2}\right)\right)\cos\left(\frac{\sqrt{3}x}{2} + \frac{3y}{2}\right)$$

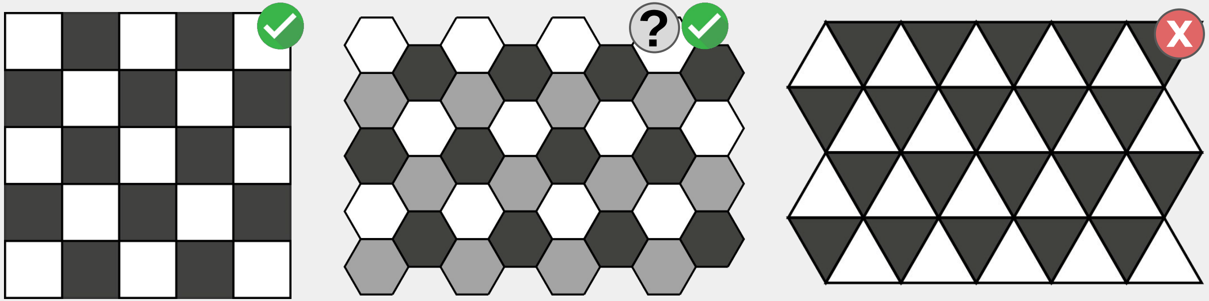




Conclusions

- Emergence of <u>stable</u> structures (**island myriads**) over <u>unstable</u> equilibrium points [1]

- *Conjecture*: Expected for any potential with **tiling symmetry**...



- Must result from a combination of **resonances + symmetry**

Acknowledgements

[1] M. Lazarotto ***et al.*** "Island myriads in periodic potentials", *Chaos*, 34, (2024)

[2] M. Lazarotto ***et al.*** "Diffusion transitions in a 2D periodic lattice", *CNSNS*, 112, (2022)


The End

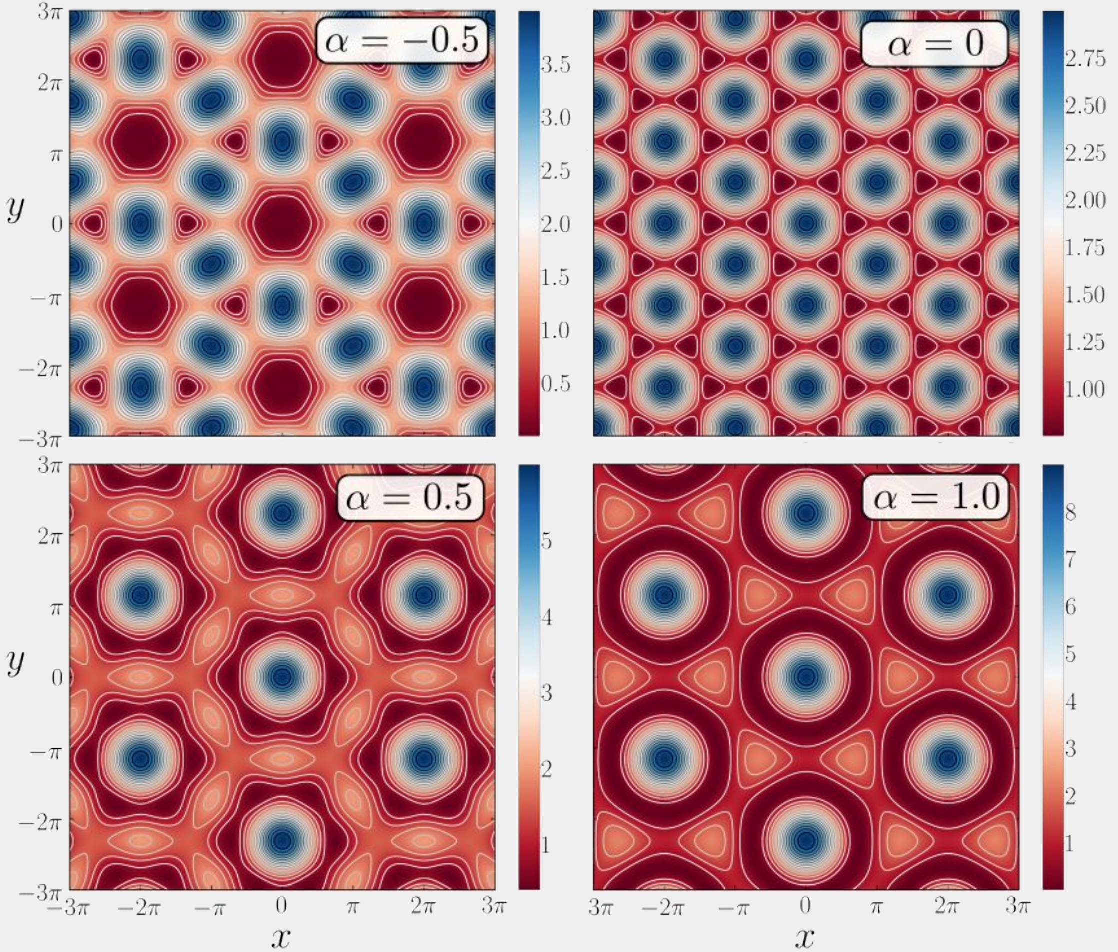
Appendix

Honeycomb potential – single coupling

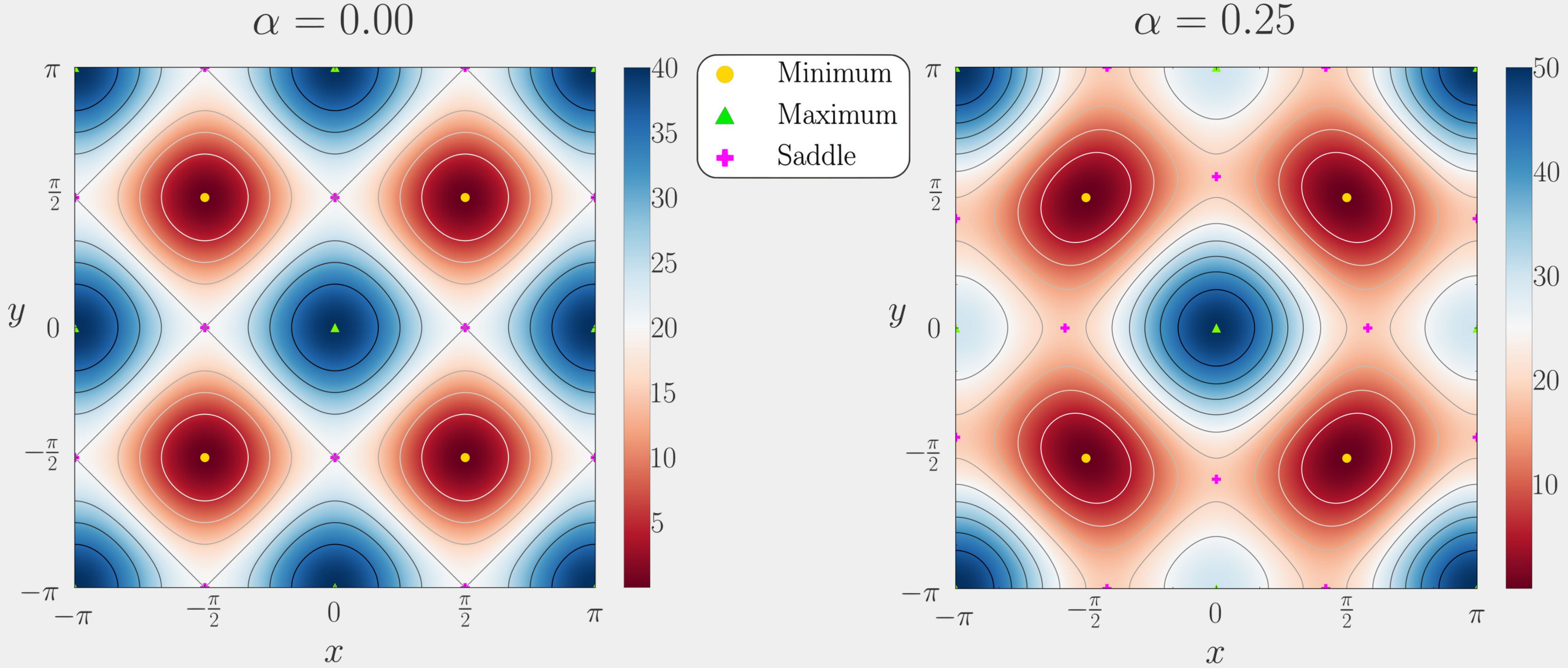
- Hexagonal unit cell
- Single coupling condition:
  - Geometrical restriction:

$$\alpha \in \left[-\frac{1}{2},\ 1\right]$$

  - Reduction of parameter space
  - Transformations keep equilibrium points fixed in space and preserve hexagonal symmetry

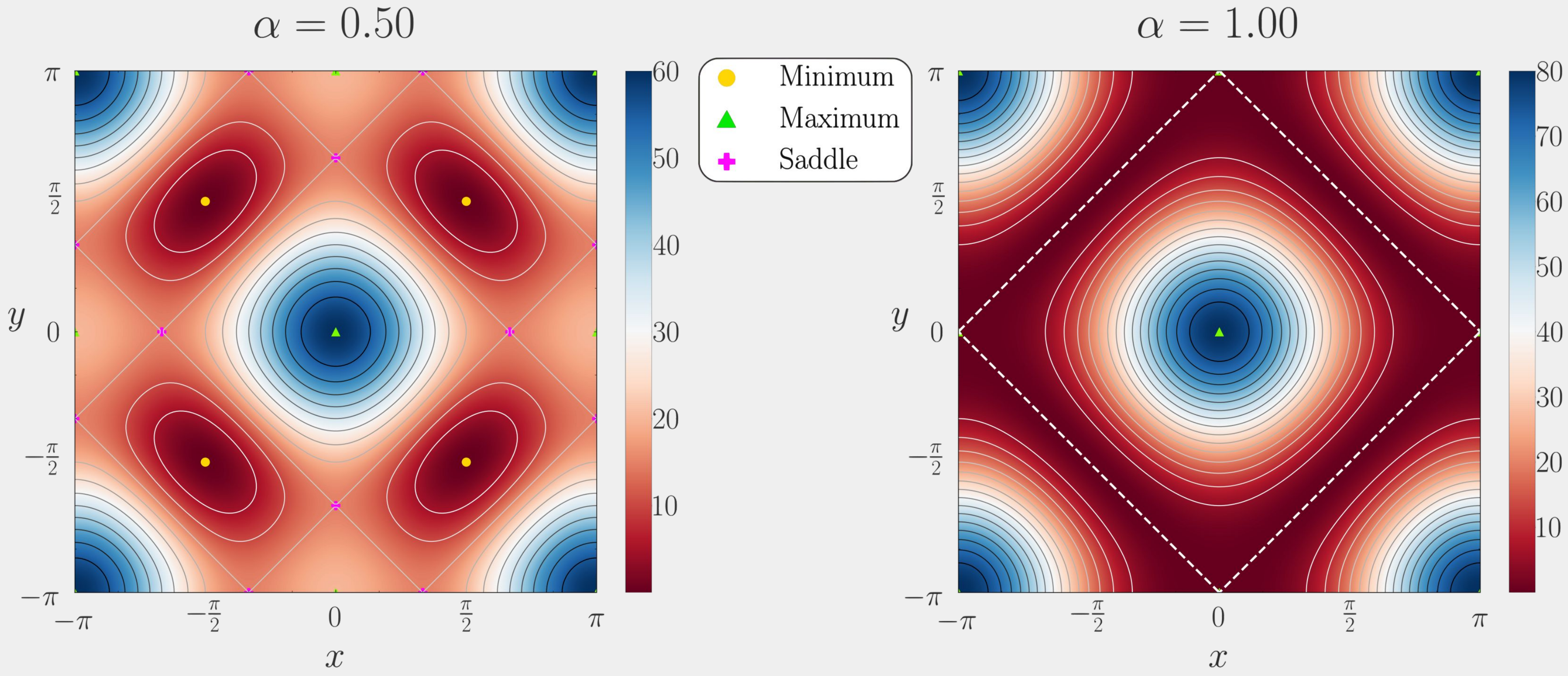


$$V(x,y) = U\left(\cos^2(x) + \cos^2(y) + 2\alpha\cos(x)\cos(y)\right)$$



- Symmetric under **rotations**:
  $\left(\frac{n\pi}{2}, n \in \mathbb{Z}\right)$
- Symmetric under **translations**:
  $(2m\pi,\ m \in \mathbb{Z})$

$$V(x, y) = U\left(\cos^2(x) + \cos^2(y) + 2\alpha\cos(x)\cos(y)\right)$$

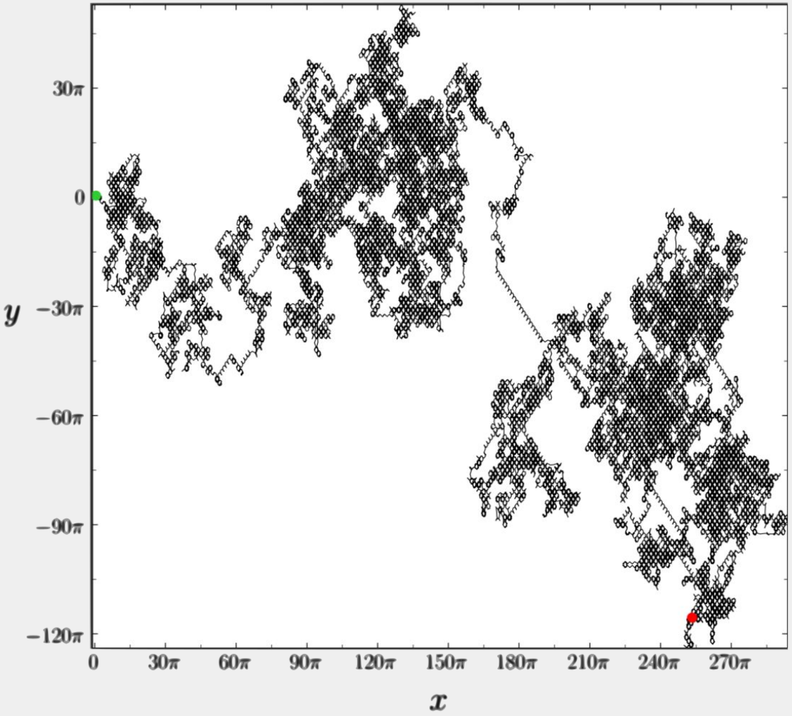


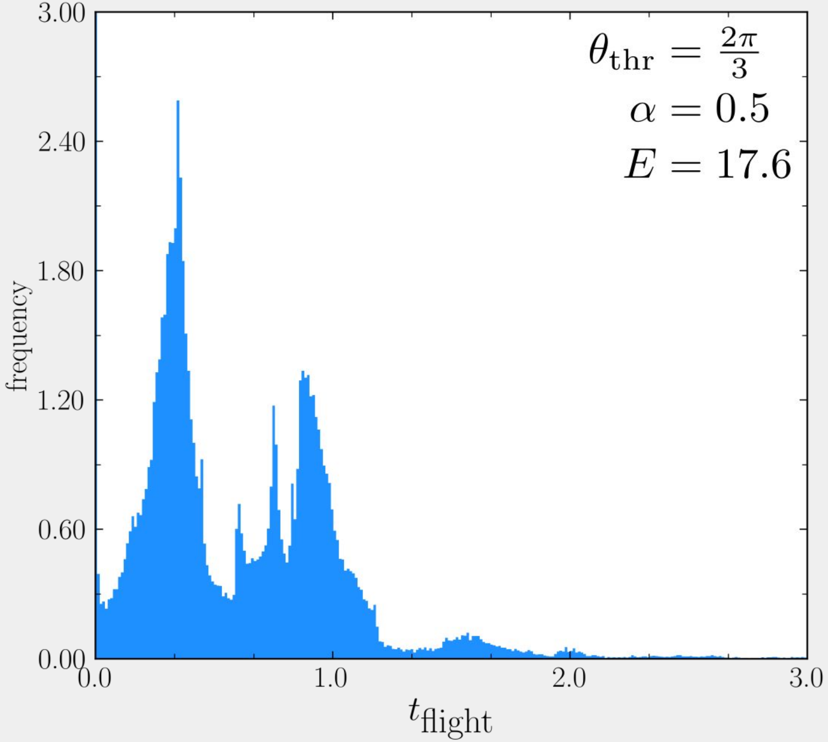
- Global **maxima** and **minima** points remain fixed as α changes.
- At $\alpha = 1.0$, saddle and local maxima merge (minimum trench line)

Diffusion trajectories

- Short range chaotic displacement $\longrightarrow$ tens or hundreds of lattice cells

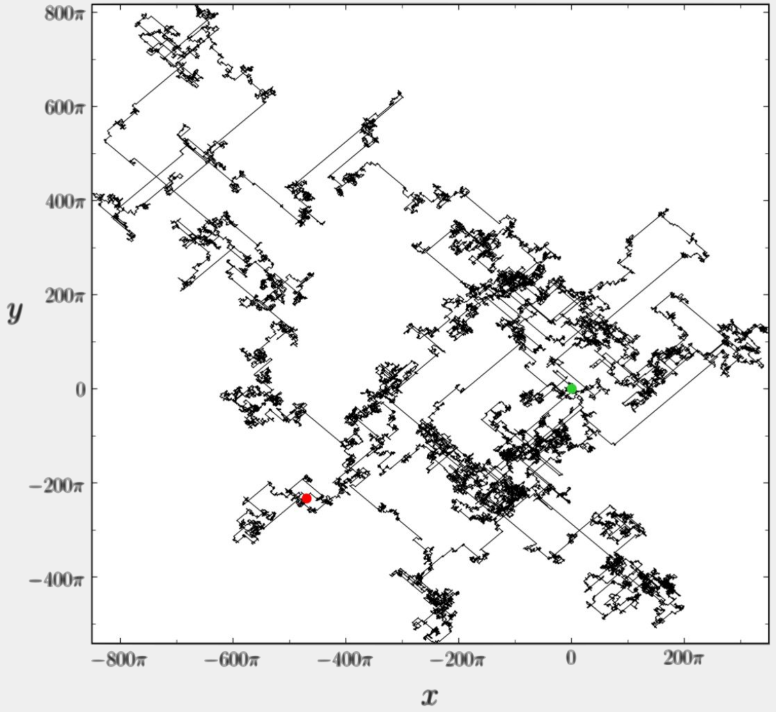
- Normal diffusion regime $\mu \approx 1$



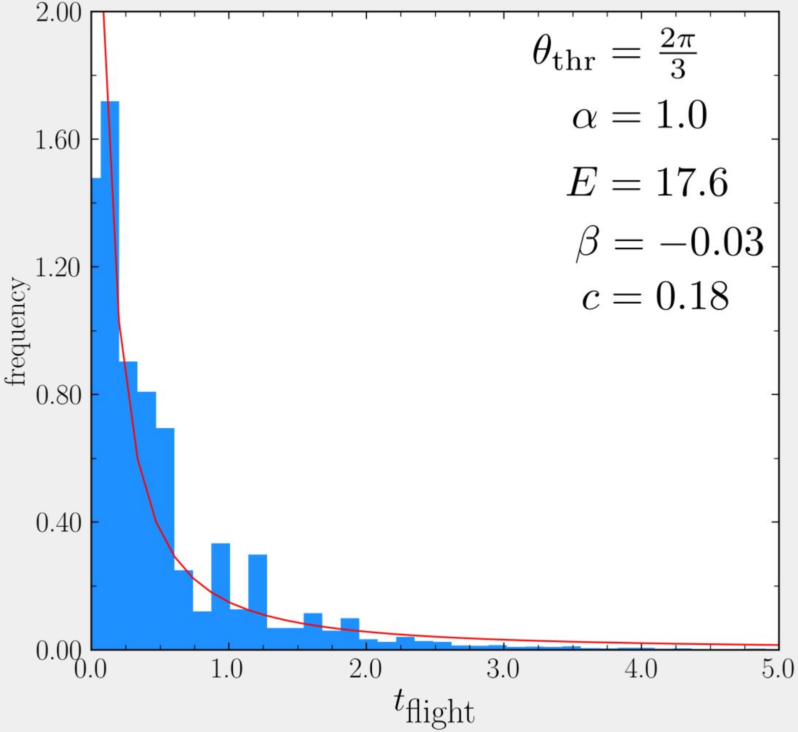


Diffusion trajectories

- Long range chaotic displacement (Lévy flights) $\longrightarrow$ a thousand lattice cells
- Free diffusion regime $\mu \approx 2$

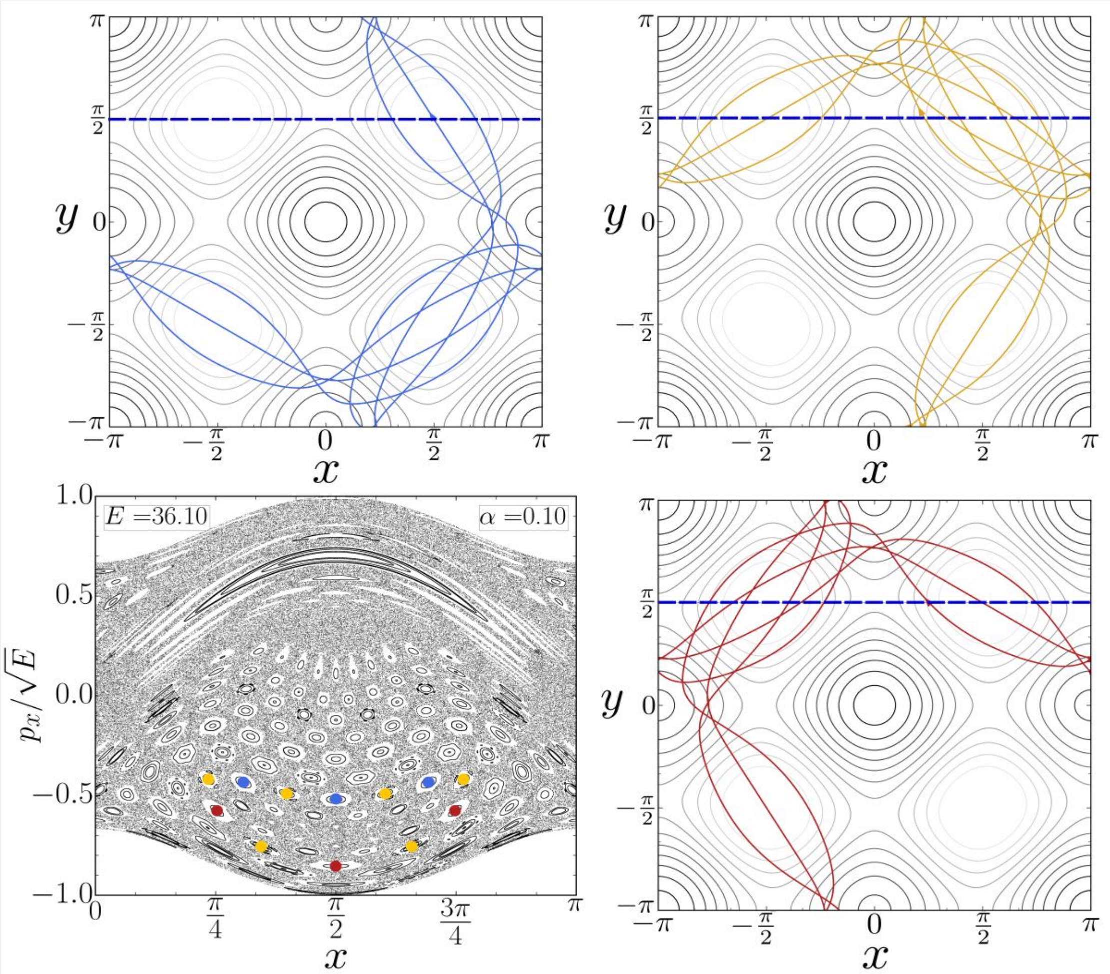


$$f(x) = \sqrt{\frac{c}{2\pi(x-\beta)^3}}\, e^{-\frac{c}{2(x-\beta)}}$$

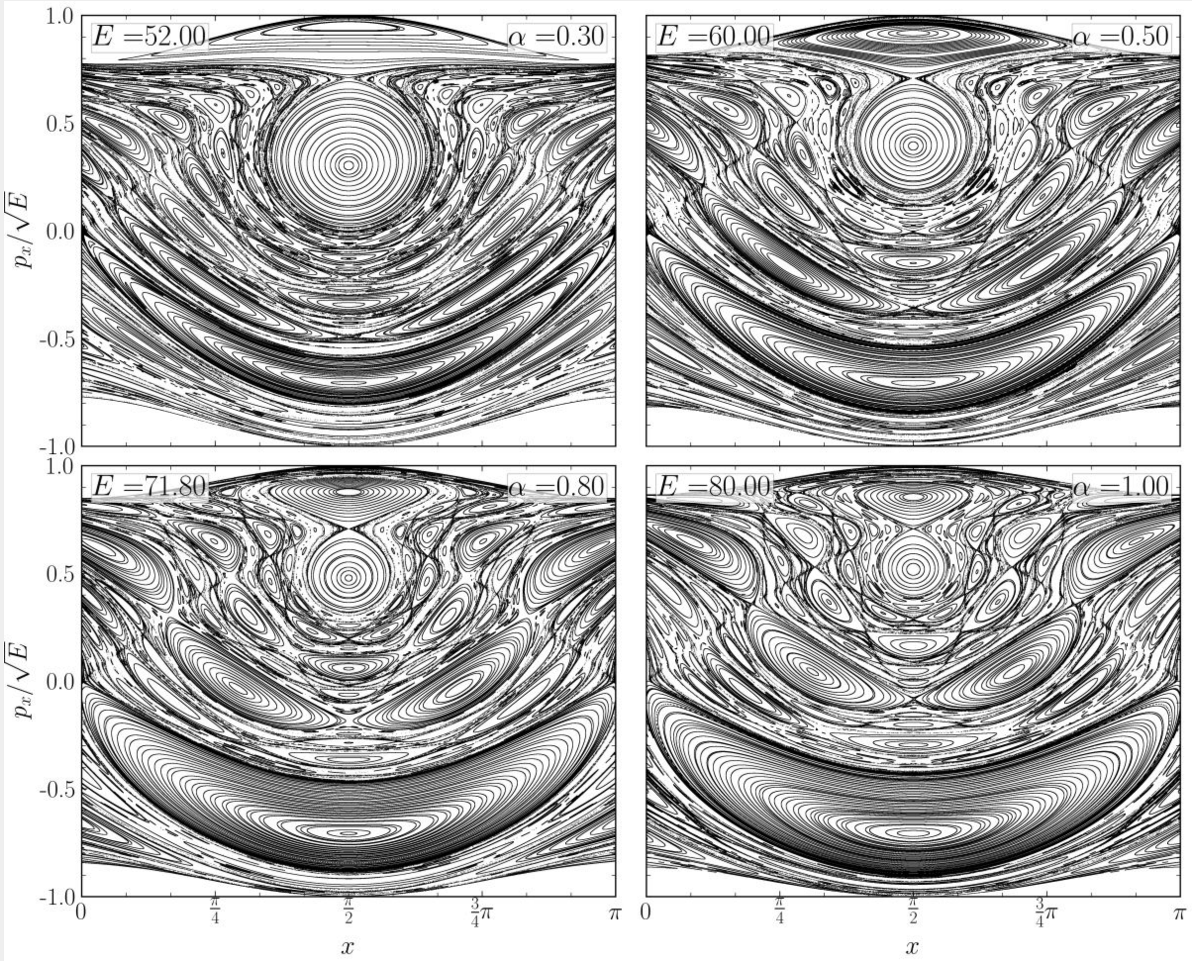


Appendix – Isochronous chains with higher multiplicity

- Isochronous chain with single period **12**
- Three-fold isochronicity
  - Fixed point **period 3**
  - Fixed point **period 3**
  - Fixed point **period 6**



Appendix – Island myriad near max energy



Monodromy method for numerical calculation of periodic orbits

- Excerpts from N. S. Simonovic, ‘Calculations of periodic orbits: The monodromy method and application to regularized systems’, *Chaos* **9(4)**, (1999); DOI: 10.1063/1.166457

$$\mathbf{s}(t_k) = \mathbf{s}_k = (q_{1,k} \ \cdots \ q_{n,k} \ \ p_{1,k} \ \cdots \ p_{n,k})^T$$

where the discrete time step evolution is performed as:

$$\begin{aligned} q_{i,k+1} &= q_{i,k} + \Delta t \ \partial_{p_i} H(\mathbf{p}, \mathbf{q}) = q_{i,k} + \Delta t \ \frac{p_{i,k}}{m} \\ p_{i,k+1} &= p_{i,k} - \Delta t \ \partial_{q_i} H(\mathbf{p}, \mathbf{q}) = p_{i,k} - \Delta t \ V_i(\mathbf{q}_{k+1}) \end{aligned}$$

for $i \in [0, n]$ and $k \in [0, K]$ as coordinate and time discrete step index, respectively; V_i is the partial derivative $\partial_{q_i} V(\mathbf{q})$. Taking small displacements around a solution orbit $(\mathbf{q}^0, \mathbf{p}^0)$, we have the linear form:

$$\begin{aligned} q_{i,k} = q^0_{i,k} + \delta q_{i,k} \quad &\xrightarrow{\text{linear}} \quad \delta q_{i,k+1} = \delta q_{i,k} + c'_{i,k} + \Delta t \ \frac{\delta p_{i,k}}{m} \\ p_{i,k} = p^0_{i,k} + \delta p_{i,k} \quad &\xrightarrow{\text{linear}} \quad \delta p_{i,k+1} = \delta p_{i,k} + c'_{i+n,k} - \Delta t \sum_{j=1}^{n} V_{ij}(\mathbf{q}^0_{k+1}) \delta q_{i,k+1} \end{aligned} \tag{2}$$

for

$$\begin{aligned} c'_{i,k} &= q^0_{i,k} - q^0_{i,k+1} + \Delta t \ \frac{p^0_{i,k}}{m} \\ c'_{i+n,k} &= p^0_{i,k} - p^0_{i,k+1} - \Delta t \ V_i(\mathbf{q}^0_{k+1}) \qquad \text{for} \qquad i \in [0, n] \end{aligned}$$

Simplifying system 2 to matrix form yields:

$$\mathbf{A}_{k+1}\delta\mathbf{s}_{k+1} = \mathbf{B}\delta\mathbf{s}_k + \mathbf{c}'_k$$

where

$$\mathbf{A}_{k+1} = \begin{pmatrix} \mathbf{I}_n & \mathbf{0}_n \\ \Delta t\mathbf{P}_{k+1} & \mathbf{I}_n \end{pmatrix} \qquad \mathbf{B} = \begin{pmatrix} \mathbf{I}_n & \Delta t\ \mathbf{m} \\ \mathbf{0}_n & \mathbf{I}_n \end{pmatrix}$$

for

$$\mathbf{P}_k = \begin{pmatrix} V_{11}(\mathbf{q}_k) & \cdots & V_{1n}(\mathbf{q}_k) \\ \vdots & \ddots & \vdots \\ V_{n1}(\mathbf{q}_k) & \cdots & V_{nn}(\mathbf{q}_k) \end{pmatrix} \qquad \mathbf{m}^{-1} = \begin{pmatrix} m^{-1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & m^{-1} \end{pmatrix}$$

Expressing $\delta\mathbf{s}_{k+1}$ alone, we get the system:

$$\delta\mathbf{s}_{k+1} = \mathbf{U}_k\delta\mathbf{s}_k + \mathbf{c}_k \tag{3}$$

for

$$\mathbf{U}_k = \mathbf{A}_{k+1}^{-1}\mathbf{B} = \begin{pmatrix} \mathbf{I}_k & \Delta t\ \mathbf{m}^{-1} \\ -\Delta t\ \mathbf{P}_{k+1} & \mathbf{I}_n - \Delta t^2 \mathbf{P}_{k+1}\mathbf{m}^{-1} \end{pmatrix}$$

$$\mathbf{c}_k = \mathbf{A}_{k+1}^{-1}\mathbf{c}'_k = \begin{pmatrix} c'_{1,k} \\ \vdots \\ c'_{n,k} \\ -\Delta t \sum_i^n V_{1i}(\mathbf{q}_{k+1}^0) c'_{i,k} + c'_{n+1,k} \\ \vdots \\ -\Delta t \sum_i^n V_{ni}(\mathbf{q}_{k+1}^0) c'_{i,k} + c'_{2n,k} \end{pmatrix}$$

Successively applying equation 3 from a initial displacement $\delta \mathbf{s}_1$ yield the k-th iteration:

$$\delta \mathbf{s}_{k+1} = \mathbf{\Lambda}_{k+1} \delta \mathbf{s}_1 + \mathbf{\Gamma}_{k+1} \tag{4}$$

$$
\begin{aligned}
\mathbf{\Lambda}_{k+1} &= \mathbf{U}_k \mathbf{\Lambda}_k && (\mathbf{\Lambda}_1 = \mathbf{I}_{2n}) \\
\mathbf{\Gamma}_{k+1} &= \mathbf{U}_k \mathbf{\Gamma}_k + \mathbf{c}_k && (\mathbf{\Gamma}_1 = \mathbf{0}_{2n})
\end{aligned}
$$

From all the possible solutions to system 4, we look for the periodic ones, that is, those whose after $K+1$ steps go back to its initial point:

$$
\delta \mathbf{s}_{K+1} = \mathbf{\Lambda}_{K+1} \delta \mathbf{s}_1 + \mathbf{\Gamma}_{K+1} \qquad \text{for} \qquad \mathbf{\Lambda}_{K+1} = \mathbf{U}_K \cdots \mathbf{U}_1 \tag{5}
$$

As shown in the previous section, the matrix $\mathbf{\Lambda}_{K+1}$ will then be the monodromy $\mathbf{M}$ in case the orbit is the periodic solution, but in its discretized form. The Newton-Raphson fashion algorithm arises when one wants to solve system 4 for $\mathbf{\Gamma}_{K+1} = \mathbf{0}_{2n}$, in order to get a periodic orbit ($\delta \mathbf{s}_{K+1} = \delta \mathbf{s}_1 = \mathbf{M} \delta \mathbf{s}_1$).

The linear equation system to be solved is then:

$$
(1 - \mathbf{\Lambda}_{K+1})\, \delta \mathbf{s}_1 = \mathbf{\Gamma}_{K+1} \tag{6}
$$

3 Calculation of periodic orbits – constant energy

The monodromy algorithm previously shown consider a fixed time step Δt and number of steps K. However, it can be desired to perform the calculation keeping the energy constant instead of the period. Thereunto, the monodromy algorithm must include a variation for the time step either $\Delta t = \Delta t^0 + \delta\Delta t$. The full discretized equations now are:

$$\delta q_{i,k+1} = \delta q_{i,k} + c'_{i,k} + \Delta t\,\frac{\delta p_{i,k}}{m} + \frac{p^0_{i,k}}{m}\delta\Delta t$$

$$\delta p_{i,k+1} = \delta p_{i,k} + c'_{i+n,k} - \Delta t\sum_{j=1}^{n} V_{ij}(\mathbf{q}^0_{k+1})\delta q_{i,k+1} - V_i(\mathbf{q}^0_{k+1})\delta\Delta t$$

yielding the following linear system:

$$\delta s_{k+1} = \mathbf{U}_k\delta\mathbf{s}_k + \mathbf{d}_k\delta\Delta t + \mathbf{c}_k$$

where

$$\mathbf{d}_k = \begin{pmatrix} \frac{p^0_{1,k}}{m} \\ \vdots \\ \frac{p^0_{n,k}}{m} \\ -\Delta t \sum_i^n V_{1i}(\mathbf{q}^0_{k+1}) \frac{p^0_{i,k}}{m} - V_1(\mathbf{q}^0_{k+1}) \\ \vdots \\ -\Delta t \sum_i^n V_{ni}(\mathbf{q}^0_{k+1}) \frac{p^0_{i,k}}{m} - V_n(\mathbf{q}^0_{k+1}) \end{pmatrix}$$

and $\mathbf{U}_k$, $\mathbf{c}_k$ are the same as previous. The iterated system in its kth-iteration will be given by:

$$\delta \mathbf{s}_{k+1} = \mathbf{U}_k \delta \mathbf{s}_k + \mathbf{\Delta}_k \delta \Delta t + \mathbf{\Gamma}_k \tag{7}$$

with the following relations and initial conditions:

$$\begin{aligned} \mathbf{\Lambda}_{k+1} &= \mathbf{U}_n \mathbf{\Lambda}_k && \text{for} && \mathbf{\Lambda}_1 = \mathbf{I}_{2n} \\ \mathbf{\Delta}_{k+1} &= \mathbf{U}_n \mathbf{\Delta}_k + \mathbf{d}_k && \text{for} && \mathbf{\Delta}_1 = \mathbf{0}_{2n} \\ \mathbf{\Gamma}_{k+1} &= \mathbf{U}_n \mathbf{\Gamma}_k + \mathbf{c}_k && \text{for} && \mathbf{\Gamma}_1 = \mathbf{0}_{2n} \end{aligned}$$

$$E_1 = \sum_{i=1}^{n} \frac{p_{i,1}^2}{2m} + V\left(\mathbf{q}_1 + \frac{\Delta t}{2m}\mathbf{p}_1\right)$$

$$\text{(linearization)} \qquad \eta = \sum_{i=1}^{F} \left[\frac{p_{i,1}^0}{m}\delta p_{i,1} + V_i(\mathbf{q}_{3/2}^0)\left(\delta q_{i,1} + \frac{\Delta t^0}{2m}\delta p_{i,1} + \frac{p_{i,1}^0}{2m}\delta\Delta t\right)\right]$$

where η is the unperturbed term

$$\eta = E_1 - \sum_{i=1}^{n} \frac{p_{i,1}^0}{2m} - V(\mathbf{q}_{3/2}^0) \tag{8}$$

The time displacement can then be eliminated by:

$$\epsilon_0 \delta\Delta t = \eta - \Theta \cdot \delta\mathbf{s}_1$$

here $\epsilon_0 = \sum_{i=1}^{n} \frac{p_{i,1}^0}{2m} V(\mathbf{q}_{3/2}^0)$ and $\Theta = (\epsilon_1 \ \cdots \ \epsilon_{2n})$ with:

$$\epsilon_i = V_i(\mathbf{q}_{3/2}^0) \qquad\qquad \epsilon_{i+n} = \frac{p_{i,1}^0}{m} + \frac{\Delta t}{2m} V_i(\mathbf{q}_{3/2}^0) \qquad \text{for} \quad i = 1, ..., n$$

Eliminating $\delta\Delta t$, the final system to be solved is thus:

$$\left(\mathbf{I}_{2n} - \mathbf{\Lambda}_{K+1} + \frac{1}{\epsilon_0}\{\mathbf{\Delta}_{K+1}, \Theta\}\right)\delta\mathbf{s}_1 = \mathbf{\Gamma}_{K+1} + \frac{\eta}{\epsilon_0}\mathbf{\Delta}_{K+1} \tag{9}$$