# Context-Informed Neural ODEs Unexpectedly Identify Broken Symmetries: Insights from the Poincaré–Hopf Theorem

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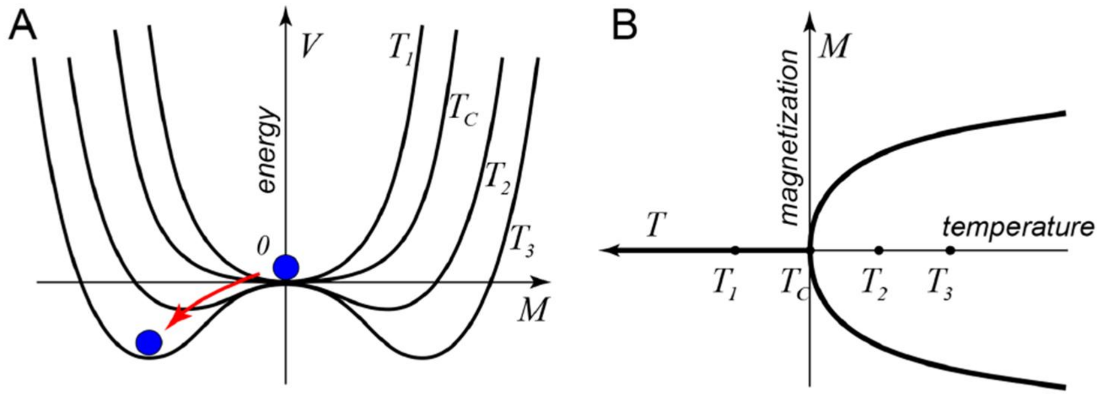
# Spontaneous Symmetry Breaking (SSB)

- SSB offers a unified framework for modeling diverse phenomena involving phase transitions.

Symmetry breaking in magnetism [1]




[1] Goryachev, A. B. et al. Molecular Biology of the Cell 2017

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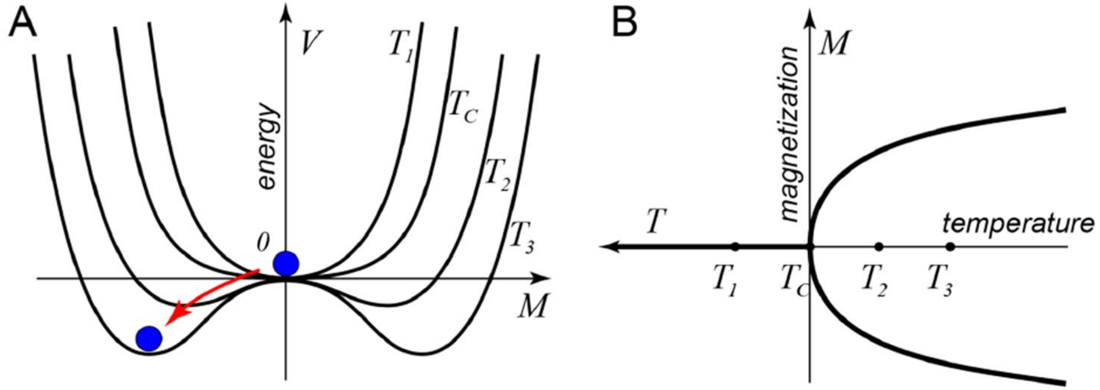
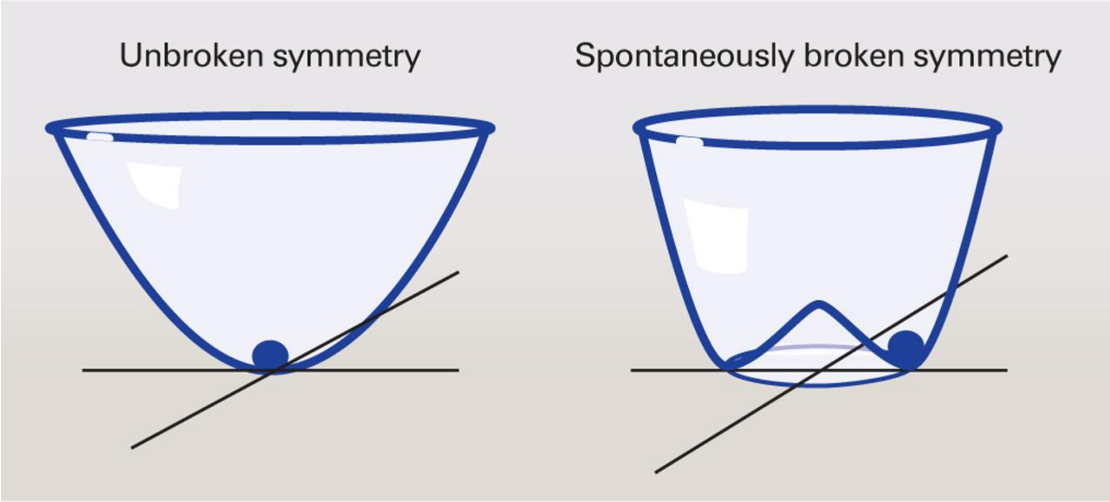



Symmetry breaking in theoretical physics [2]




[2] Cho, A. Science 2012

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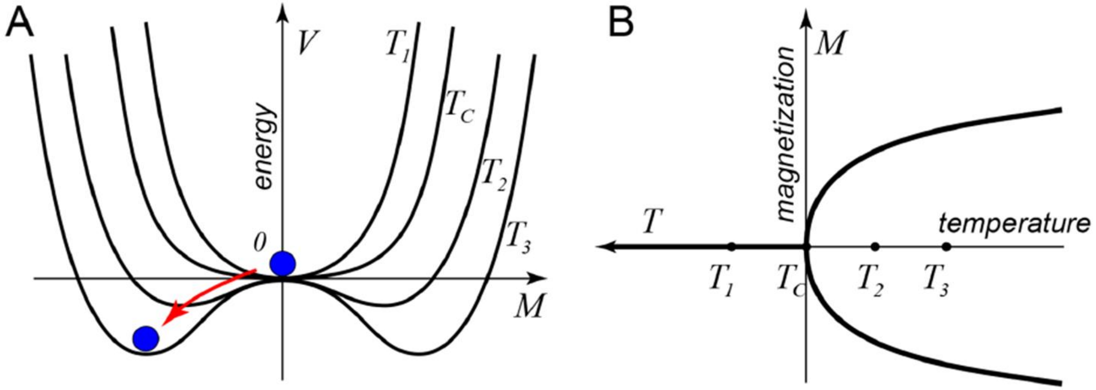


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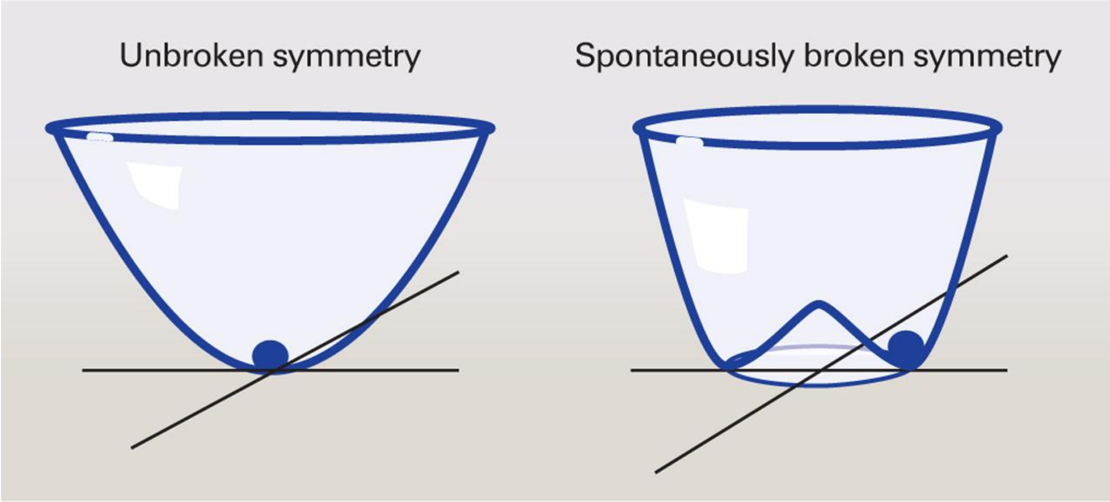
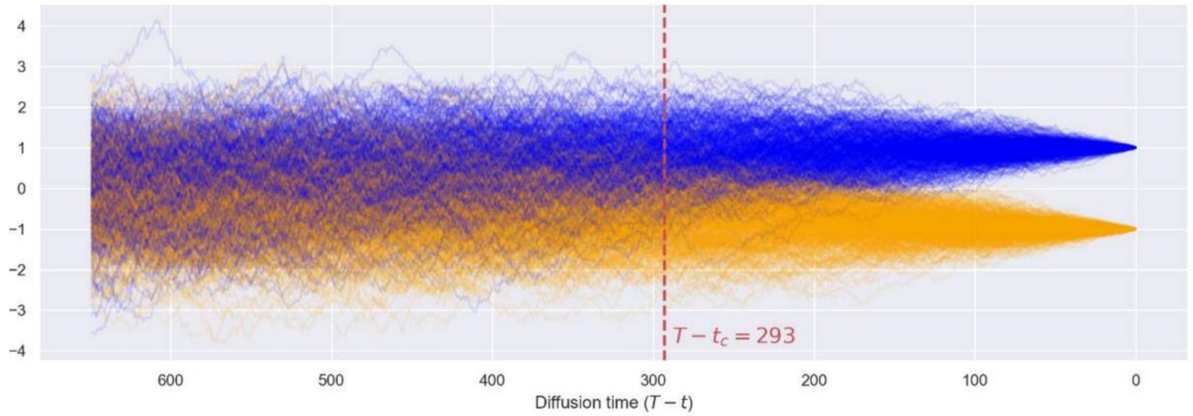
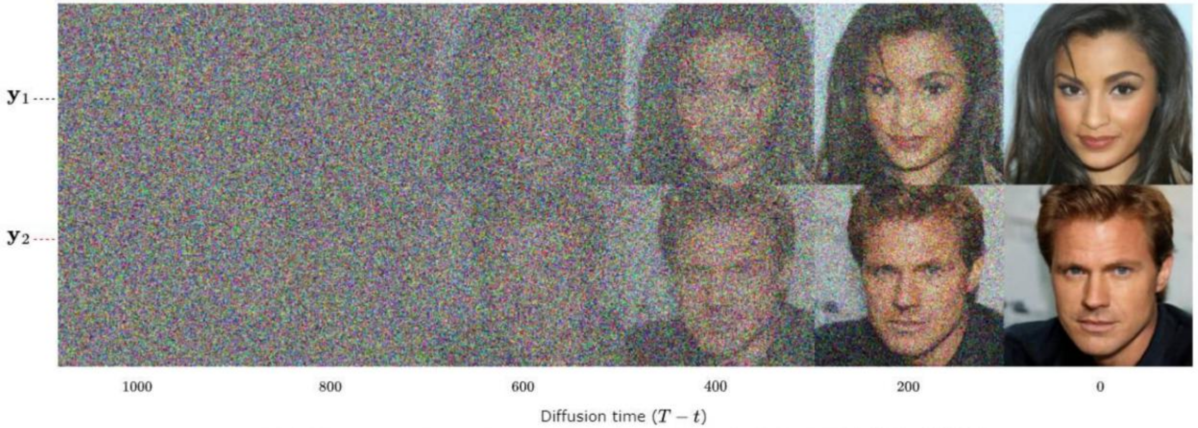



Symmetry breaking in generative models [3]




(a) Symmetry breaking in 1D diffusion model




(b) Symmetry breaking in CelebA HQ 256x256

[3] Raya, G. et al. NeurIPS 2023

# SSB as a bifurcation

- A representative example is a 2D non-linear oscillator

model parameter (= condition, environment, …)

$$\dot{\mathbf{x}} = (\dot{q}, \dot{p}) = (\partial_p \mathcal{H}, -\partial_q \mathcal{H}) = (p, \mu q - q^3)$$

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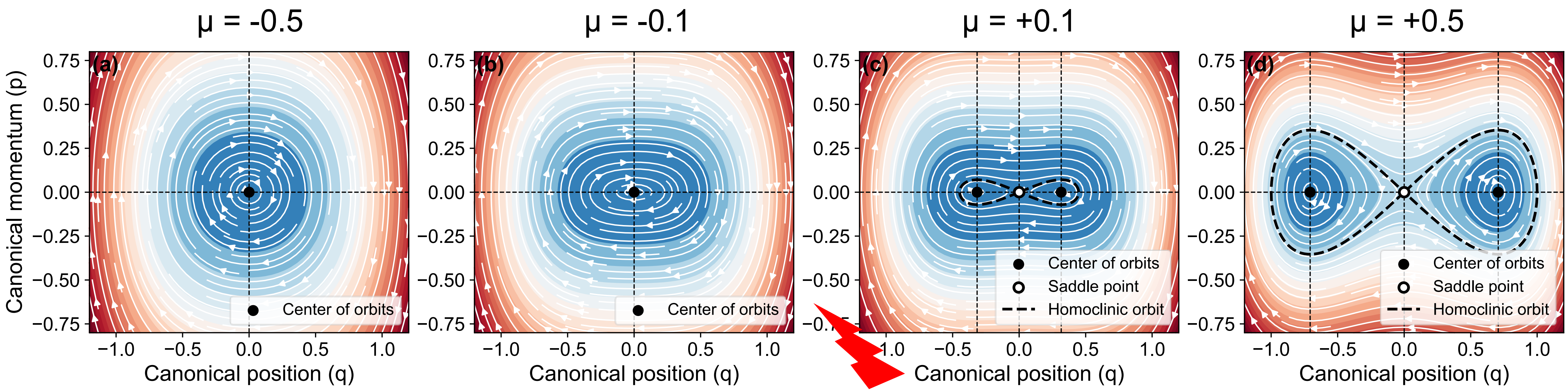


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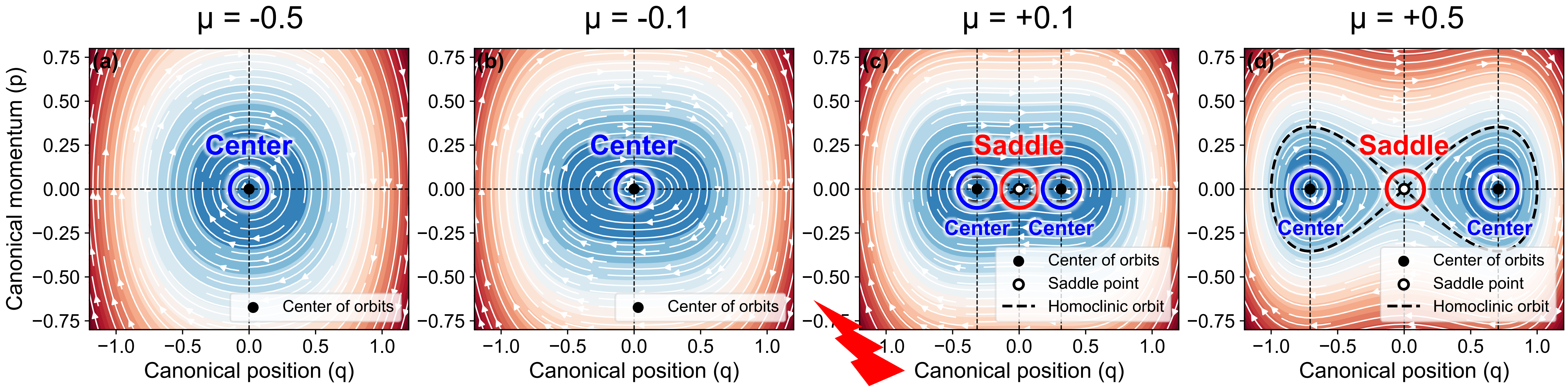


Bifurcation (@ μ = 0) from single-well to double-well dynamics!

- A symmetry-breaking bifurcation induces sudden changes in the fixed points of vector fields, altering the stability of dynamical systems (center → saddle + 2 additional centers).

# Context-Informed Neural ODEs (CI-NODEs)

- CI-NODEs [4] combine NODEs with hypernetworks to learn parameterized dynamics:

$$\tilde{\mathbf{x}}(t^j; \mathbf{x}_e^i(0), \theta_c + W\xi_e) = \mathbf{x}_e^i(0) + \int_0^{t^j} f(\tilde{\mathbf{x}}(t); \theta_c + W\xi_e)\,\mathrm{d}t$$

shared weights ($\theta_c$)

context vectors ($\xi_e$)

- Here, $\theta_c$ captures the shared information across all trajectories, while $\xi_e$ serves as an environment-specific context, analogous to the model parameter μ in physical systems.

[4] Kirchmeyer, M. et al. ICML 2022

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- In our paper, we employed CI-NODEs based on the Low-Rank Adaptation (LoRA) following [4]:

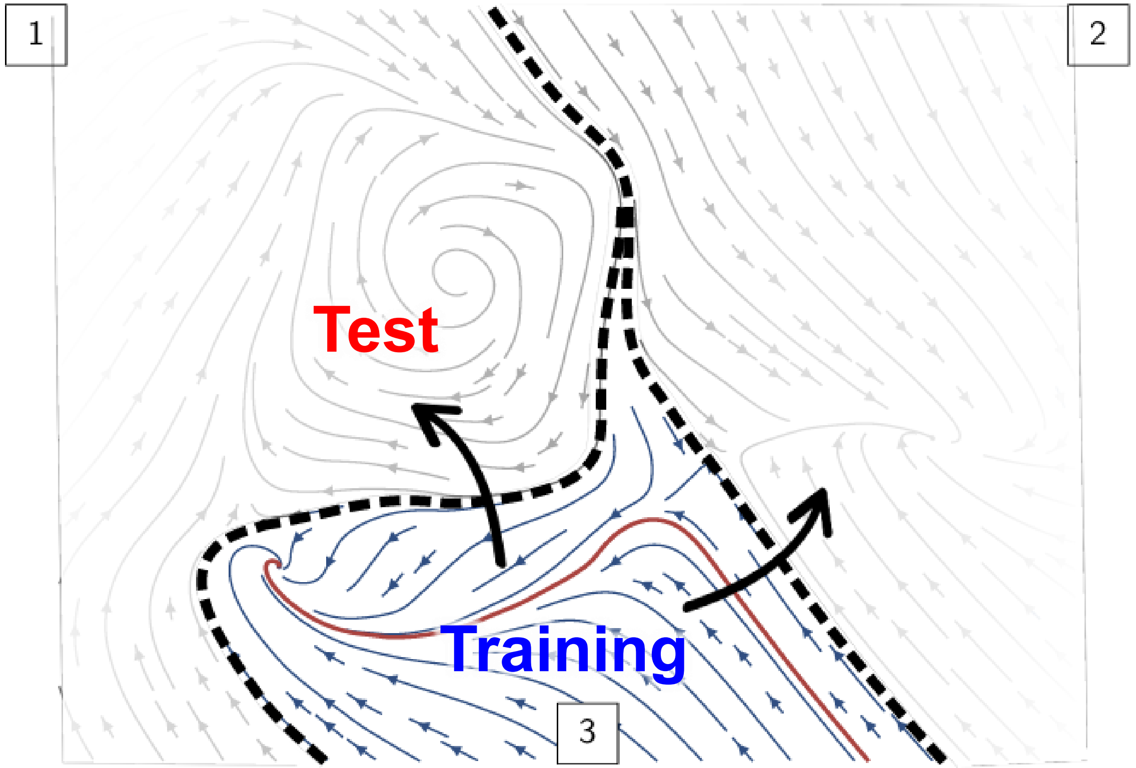
$$\theta_e = \theta(\xi_e) = \theta_c + W\xi_e \quad (\dim \xi_e \ll \dim \theta = m)$$

- There are many variants that can play a similar role with the LoRA-based CI-NODEs.
- Anyway, all of them are capable of forecasting physical systems under varying parameters by modulating the context vector ξ, either through adaptation or exploration.

[4] Kirchmeyer, M. et al. ICML 2022

# Bifurcation is another form of the Out-Of-Domain (OOD) problem

- Previous works describe OOD in dynamical systems as crossing phase space boundaries [5].




**OOD in the phase space:** Can the model trained on the third basin predict the dynamics of the first basin?

[5] Göring, N. et al. ICML 2024

# Bifurcation is another form of the Out-Of-Domain (OOD) problem

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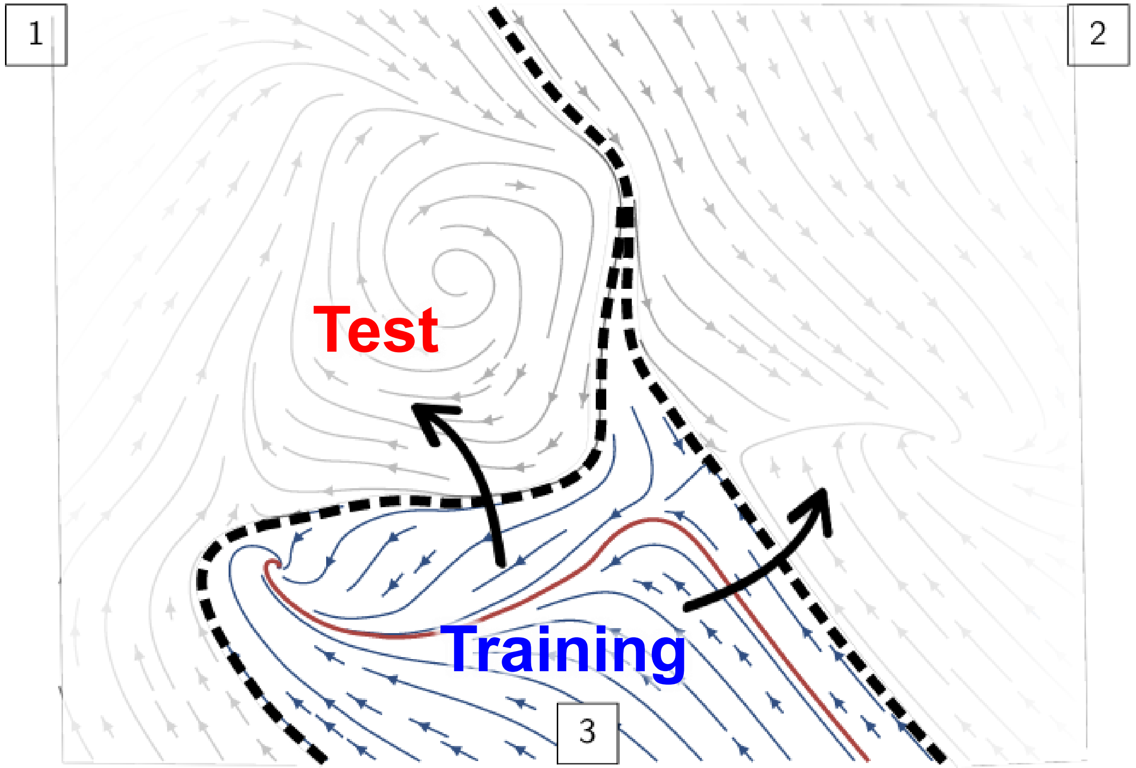
- Bifurcations can be seen as a different kind of OOD problem: crossing parameter space boundaries.

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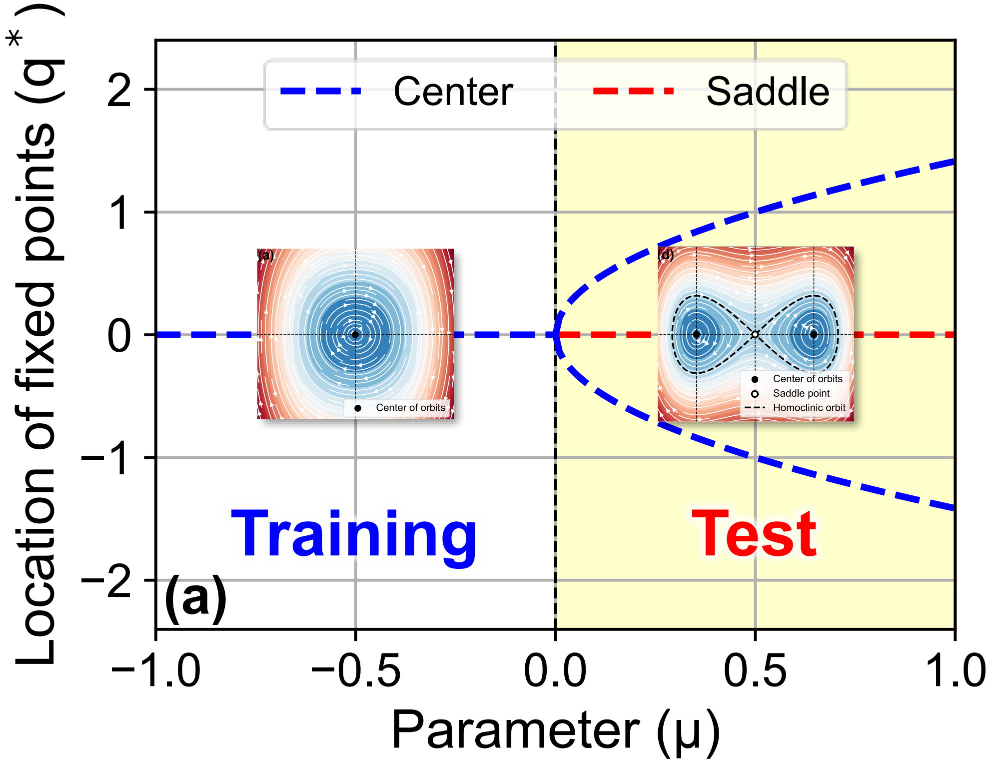
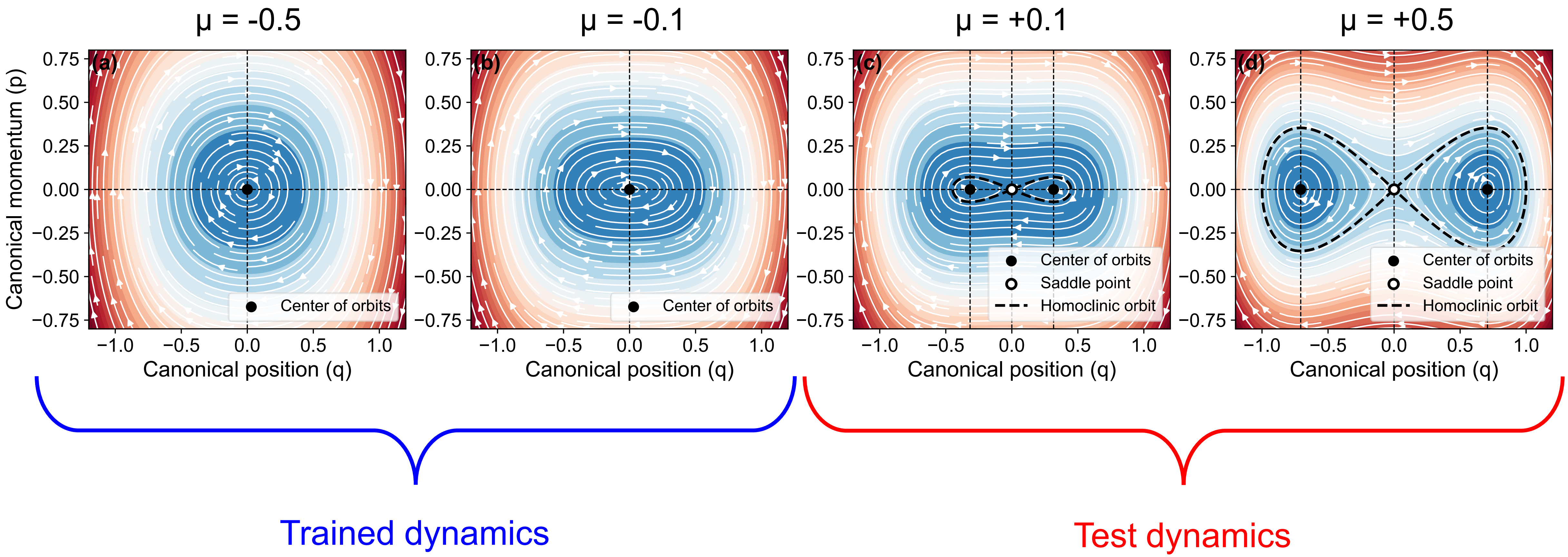



**OOD in the parameter space:** Can the model trained on μ < 0 predict the dynamics of μ > 0?

[5] Göring, N. et al. ICML 2024

# Identifying bifurcations with CI-NODEs

- Can this model forecast the post-bifurcation behavior by learning the pre-bifurcation data only?



# Identifying bifurcations with CI-NODEs

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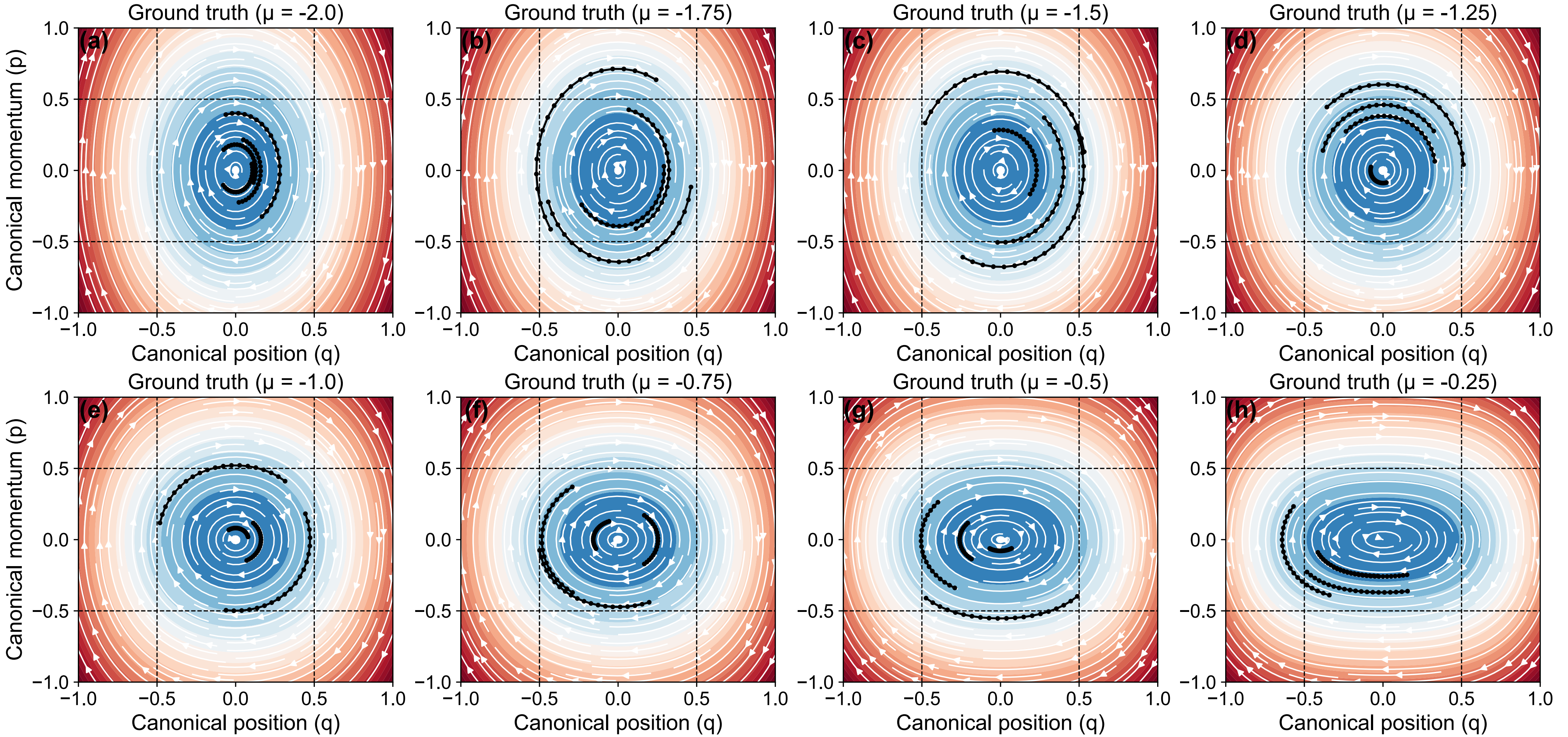
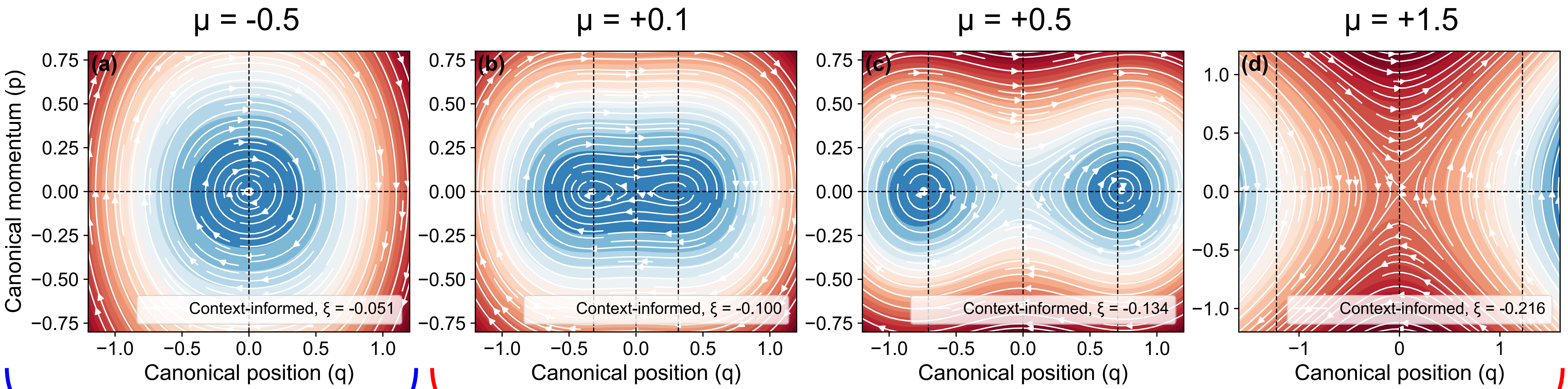
- The used training trajectories are all single-well dynamics near (0, 0) as follows:



# CI-NODEs identifies the symmetry-breaking bifurcation

- Prediction results with CI-NODEs for the 2D example:




Model prediction on the training case (μ < 0)

Model prediction on the test cases (μ > 0)

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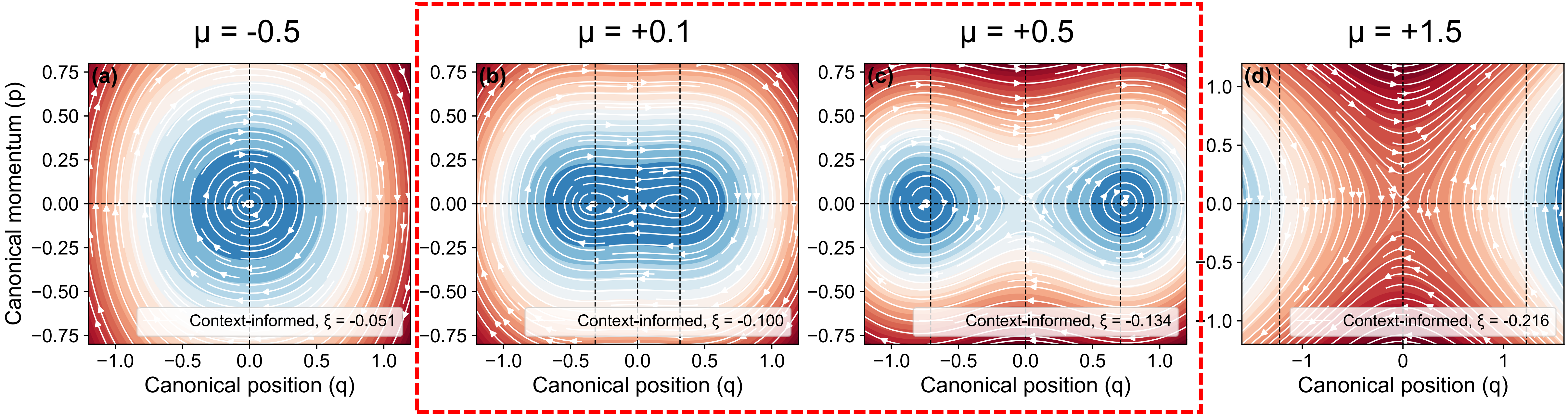


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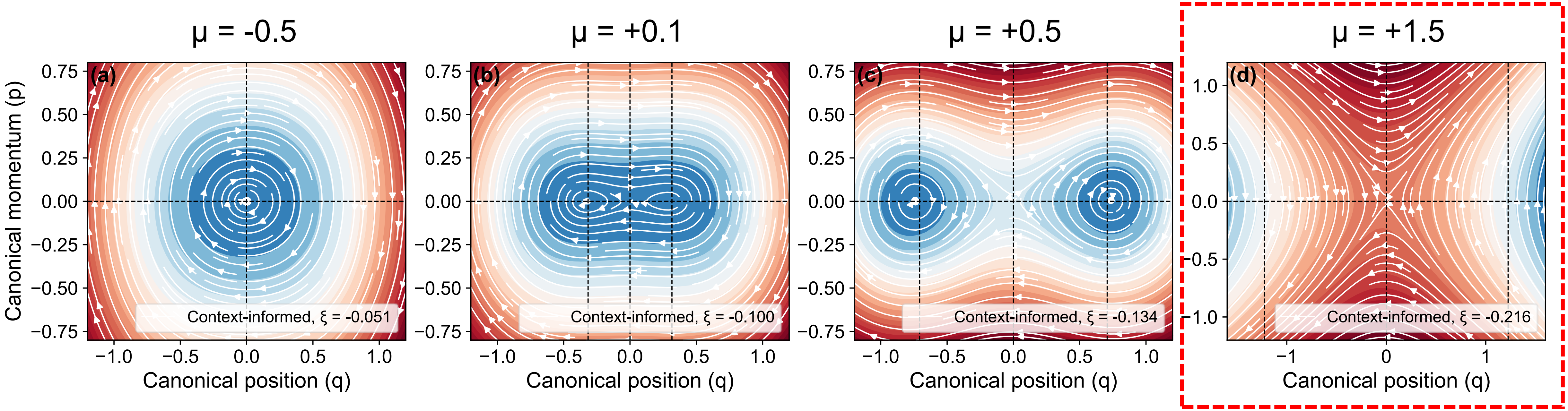


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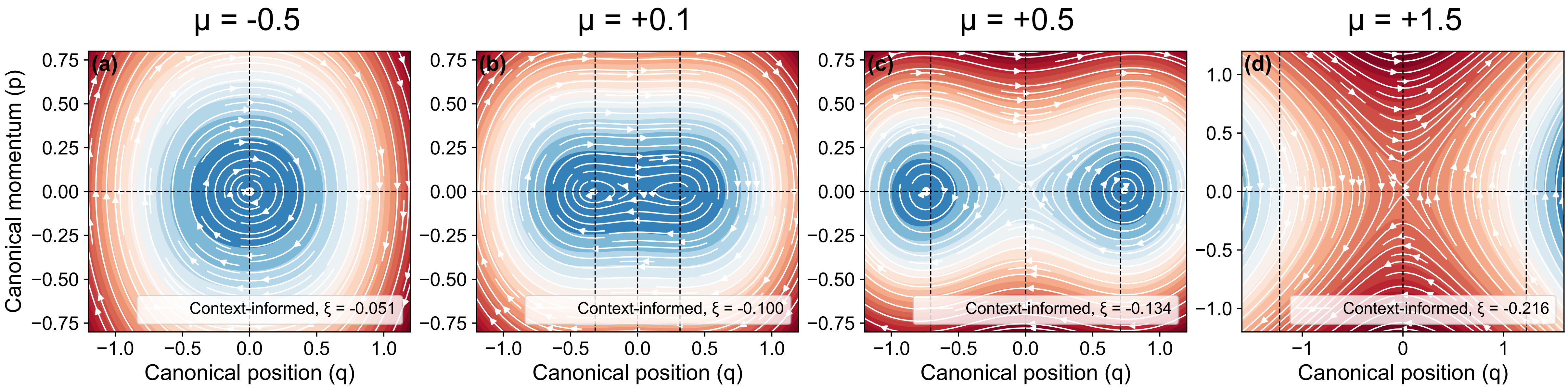
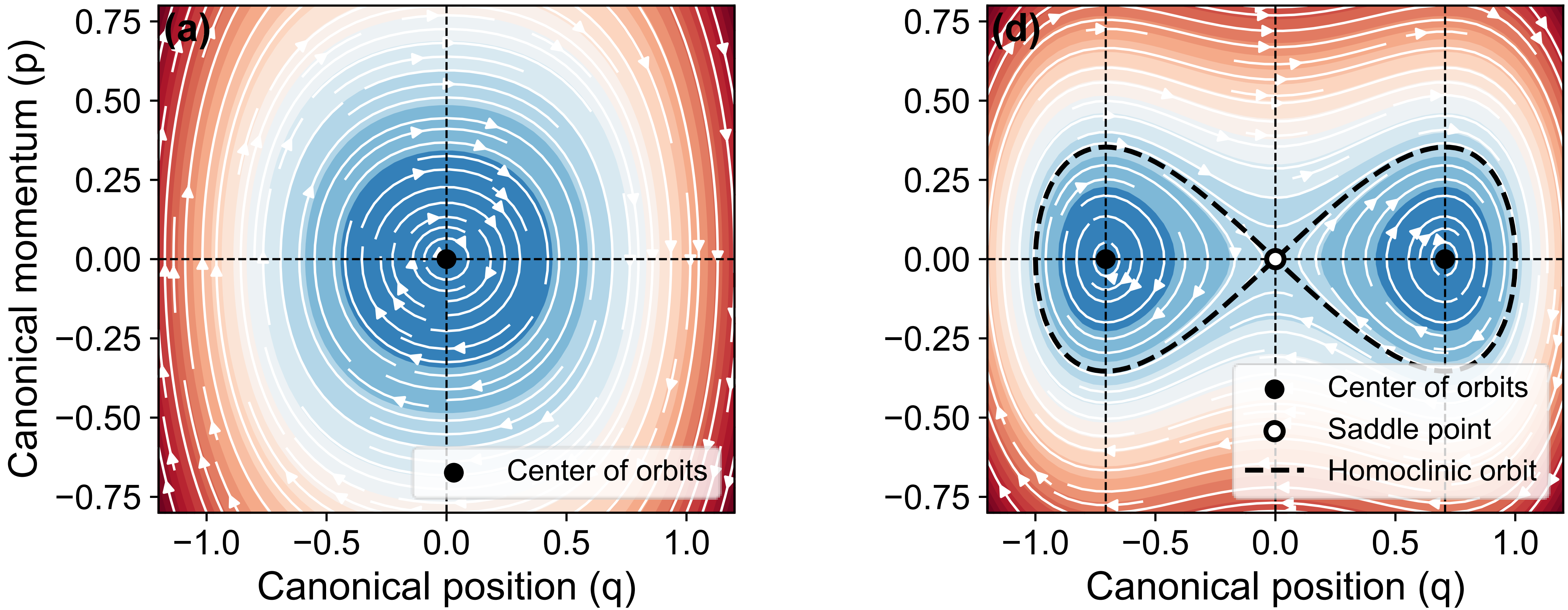



- The model identifies the double-well bifurcation near the critical point but fails to preserve its structure at higher parameter values.
- It is not surprising that the model identified the saddle transition, but how was it able to discover the symmetry-breaking double well?

# Insights from the Poincaré–Hopf theorem

- Poincaré index:

The Poincaré index is a topological number that characterizes fixed points of vector fields.



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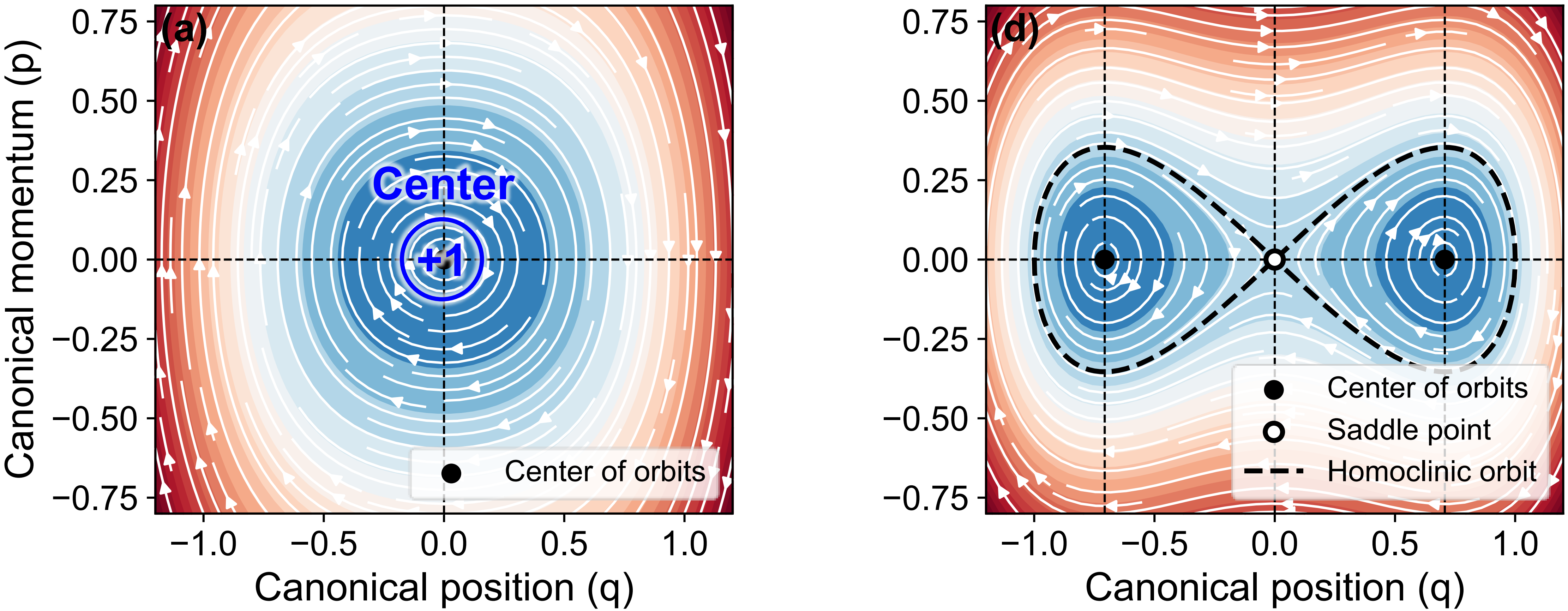

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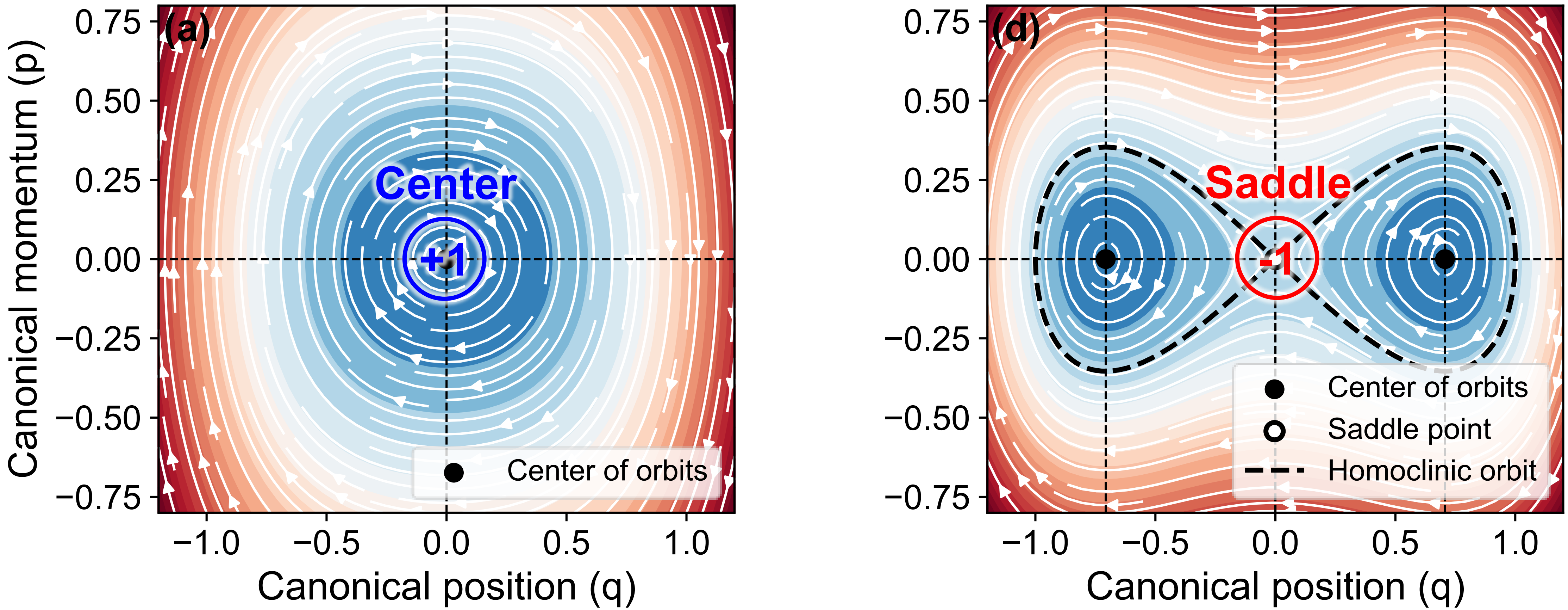

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- Poincaré–Hopf theorem:

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**Theorem 4.1.** ***(Poincaré–Hopf Theorem)*** *Let $\mathcal{M}$ be a compact, oriented, smooth manifold without boundary, and let $f : \mathcal{M} \to T\mathcal{M}$ be a smooth vector field on $\mathcal{M}$ with finitely many isolated zeros $\{\mathbf{x}_1^*, \mathbf{x}_2^*, \ldots, \mathbf{x}_k^*\}$. Then, the sum of the Poincaré indices of $f$ at these zeros is equal to the Euler characteristics $\chi(\mathcal{M})$ of $\mathcal{M}$: $\sum_{i=1}^{k} \mathrm{Ind}(f, \mathbf{x}_i^*) = \chi(\mathcal{M})$.*

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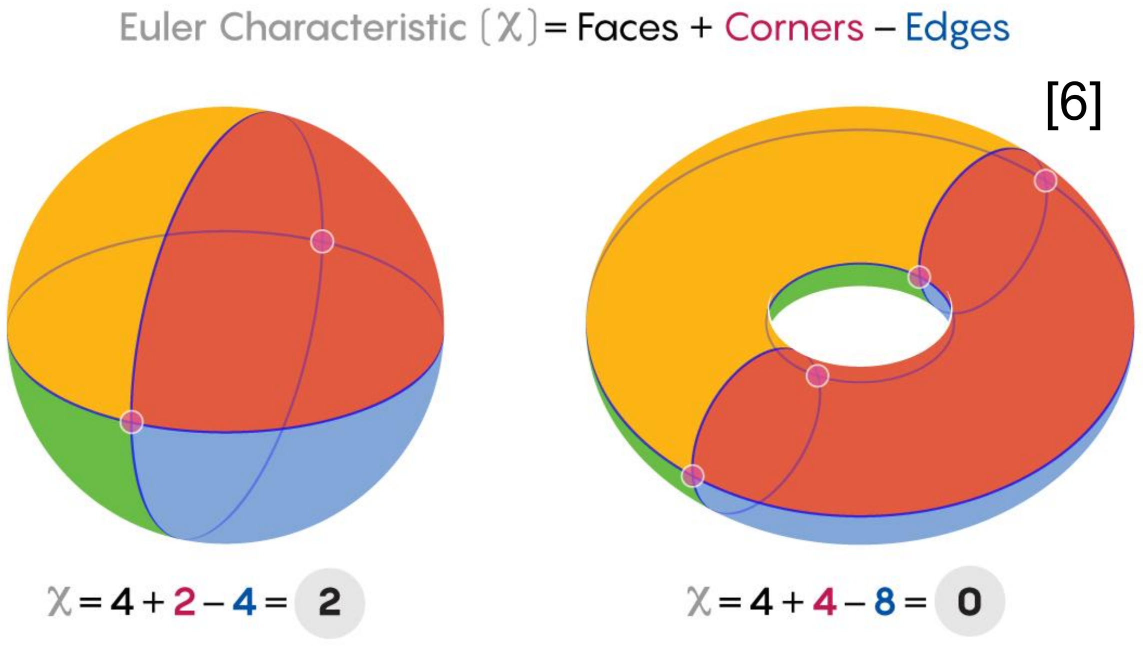


[6] Klarreich, E. Quanta Magazine 2020

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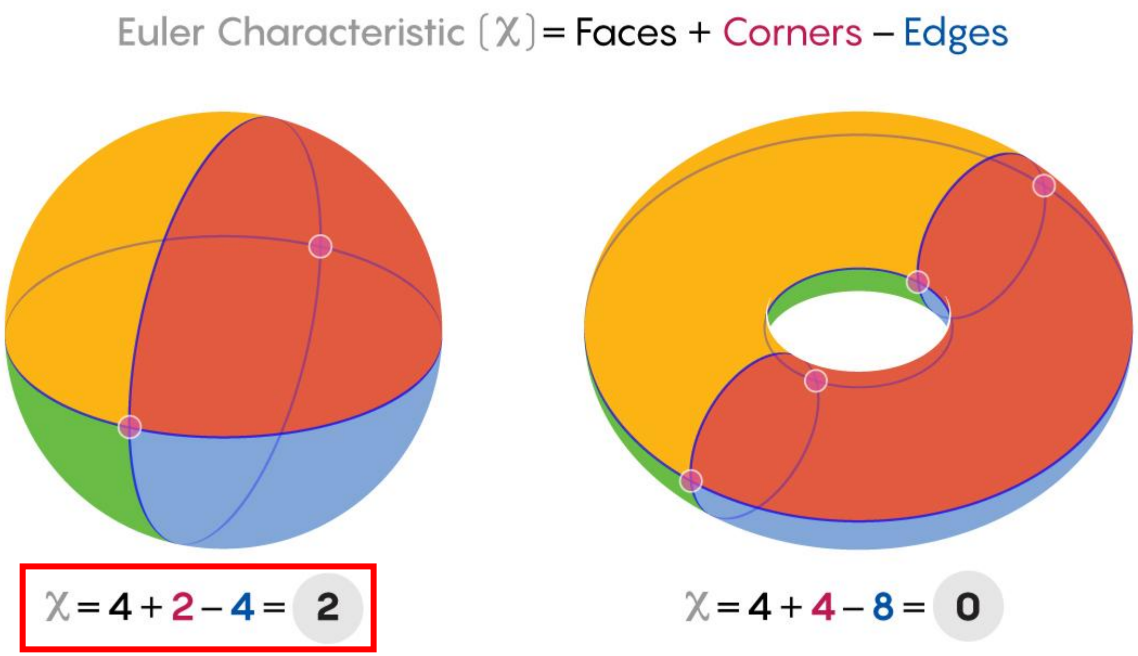


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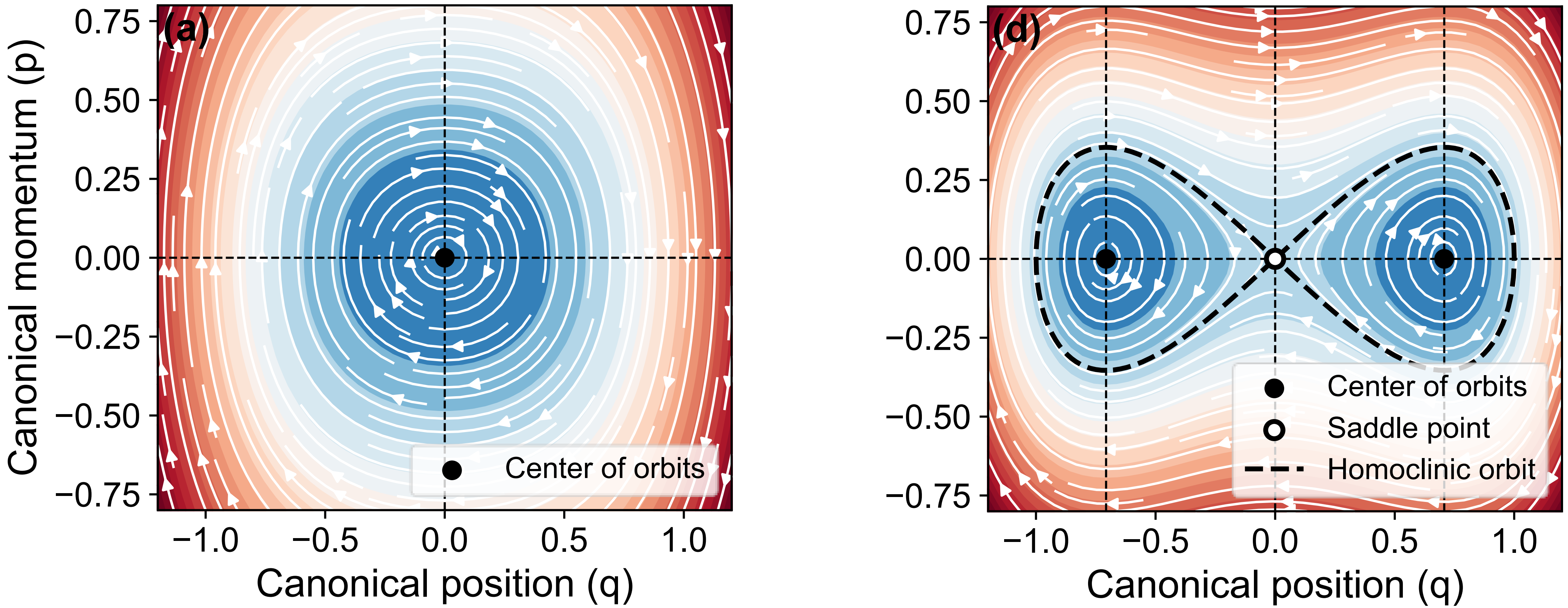
Thus, any vector field on a sphere must have a total Poincaré index of +2, thus fixed points cannot be entirely removed; unlike on a torus, where they can be.

# Insights from the Poincaré–Hopf theorem

- Poincaré–Hopf theorem (closed orbits in $\mathbb{R}^2$):

In a system bounded by a closed orbit, the sum of the indices of all enclosed fixed points must equal +1.



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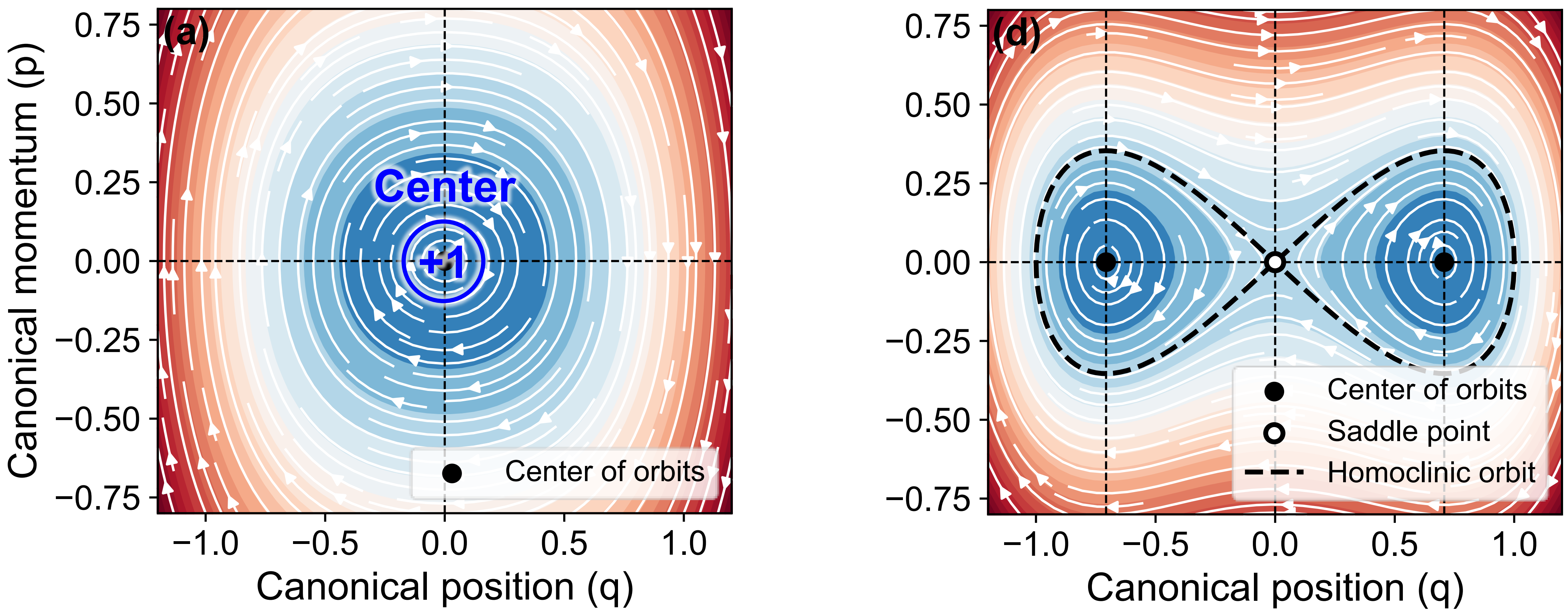

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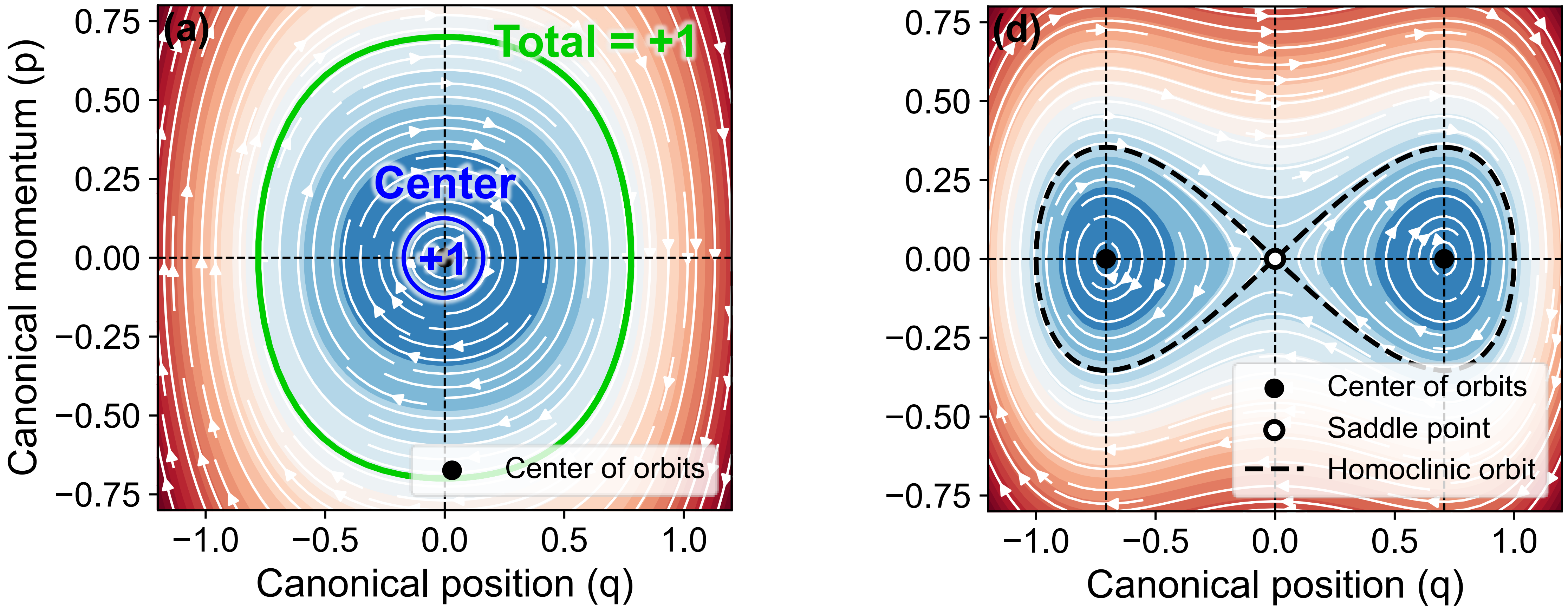

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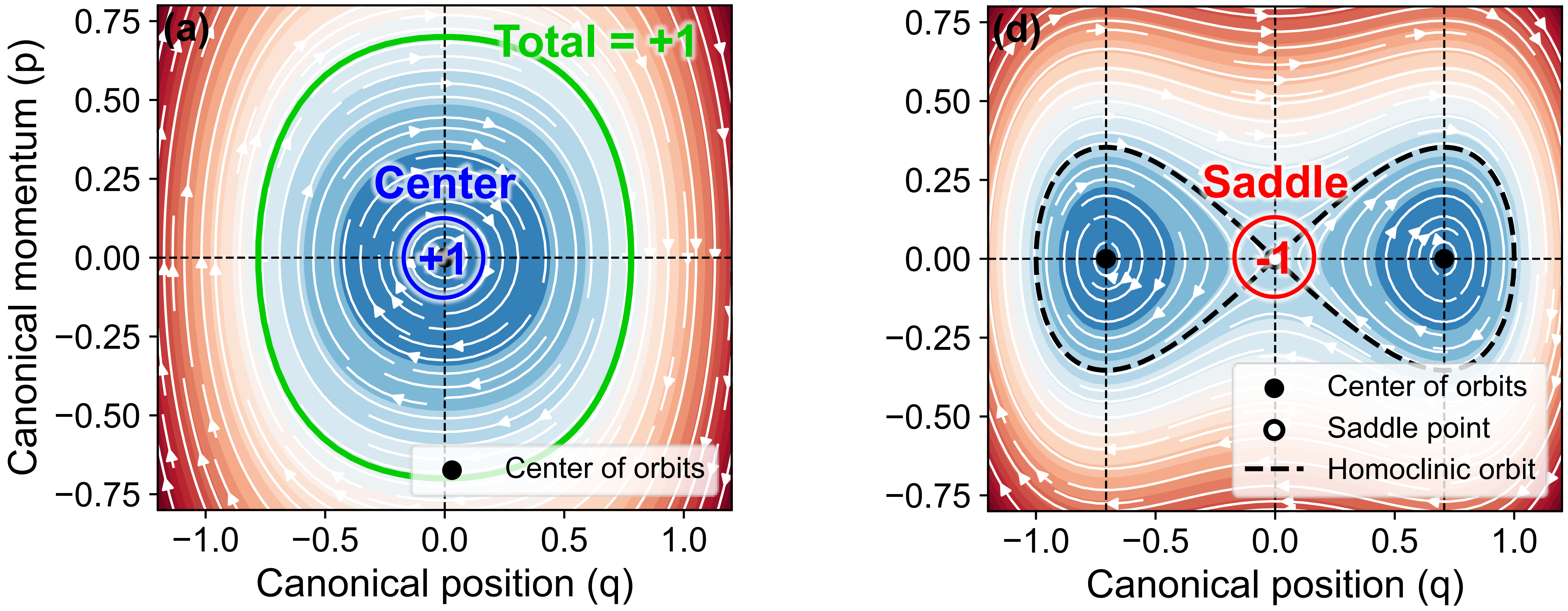

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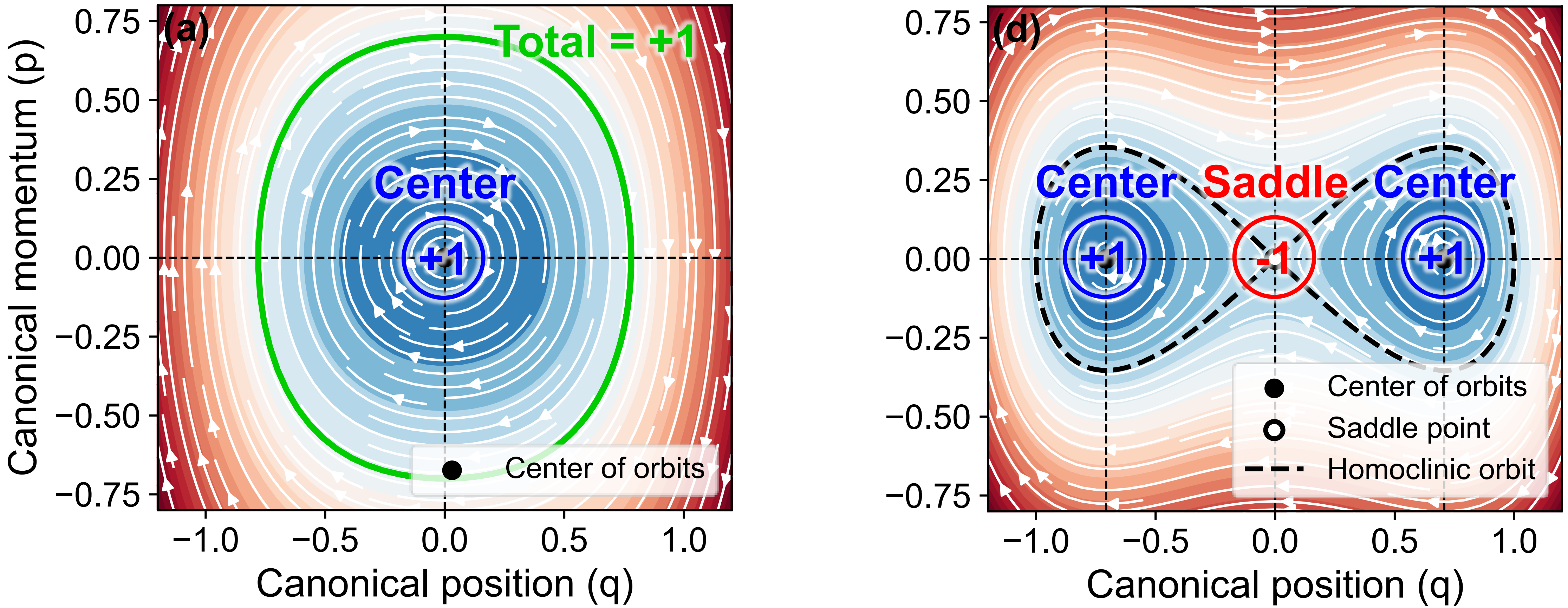

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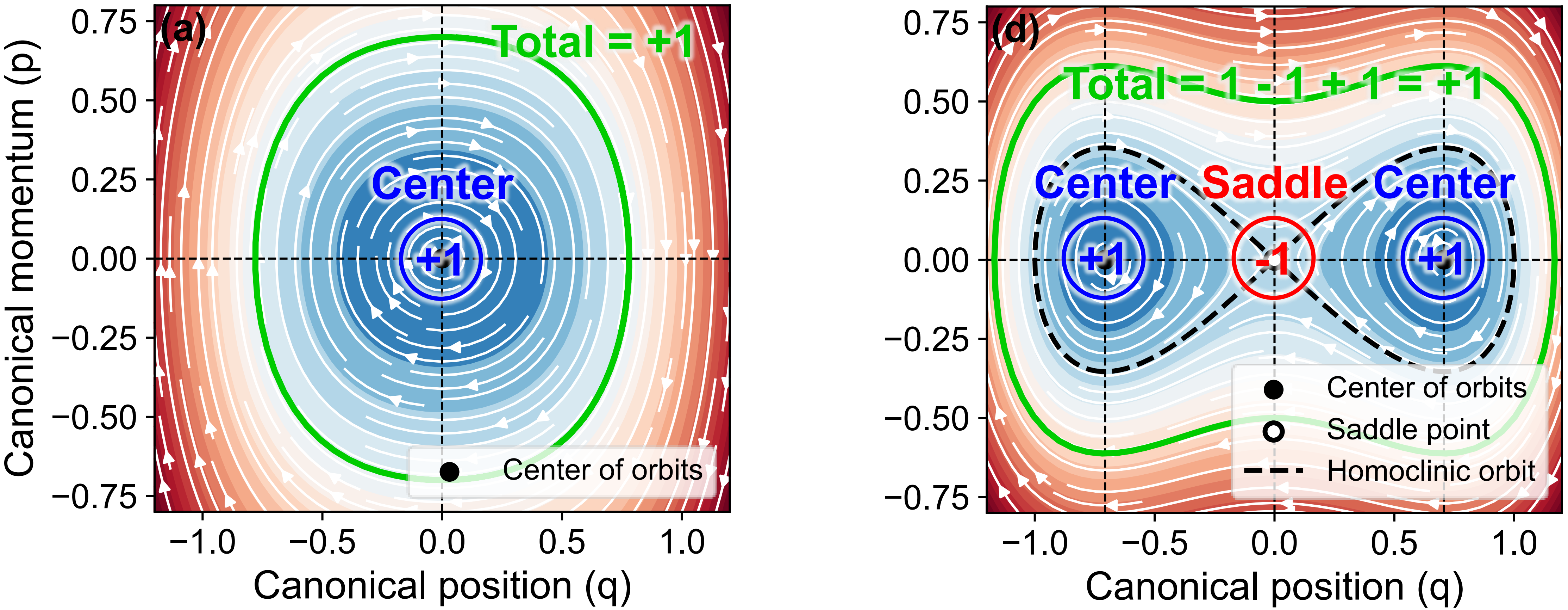

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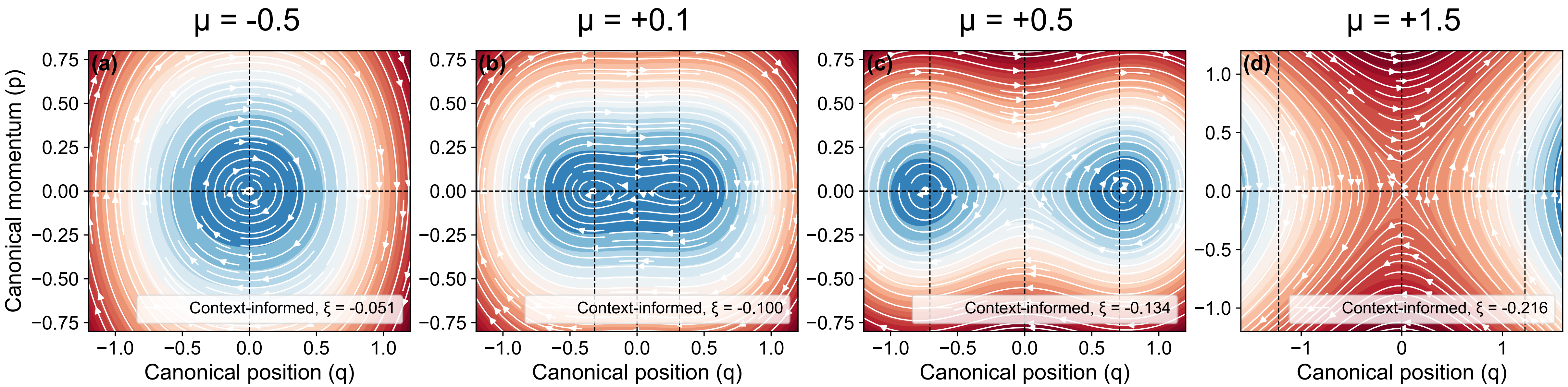

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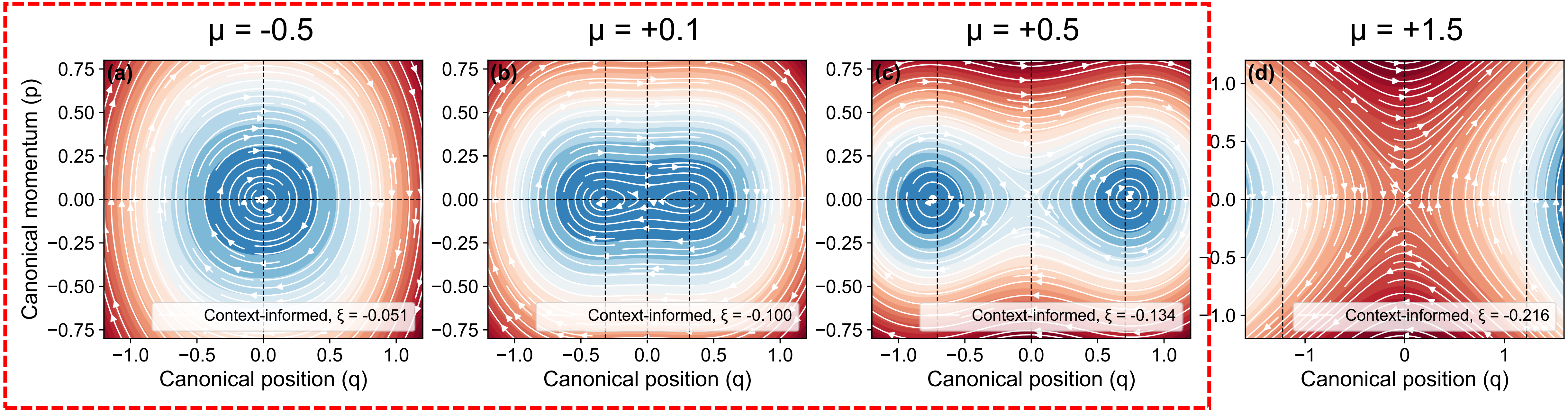

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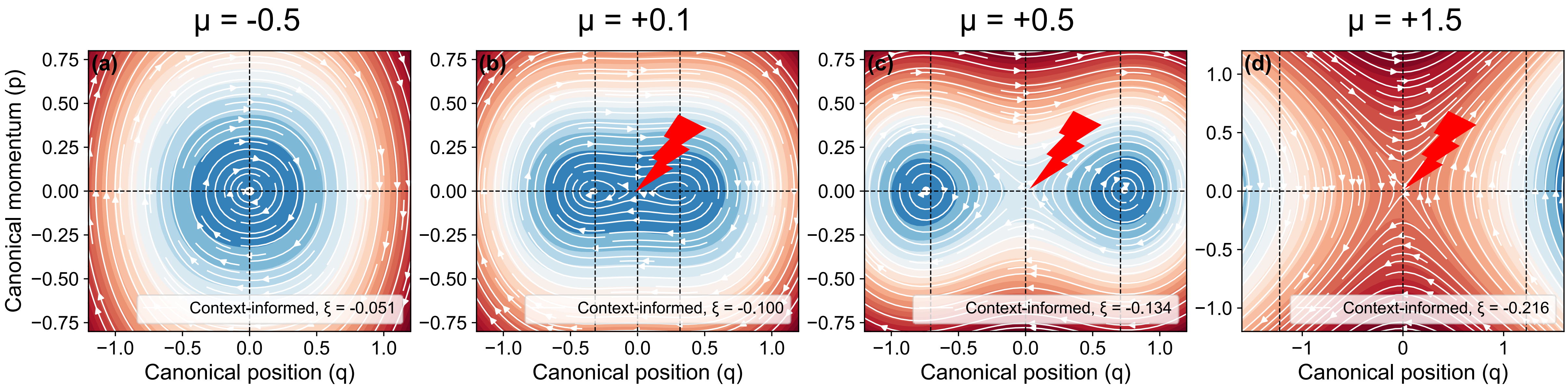

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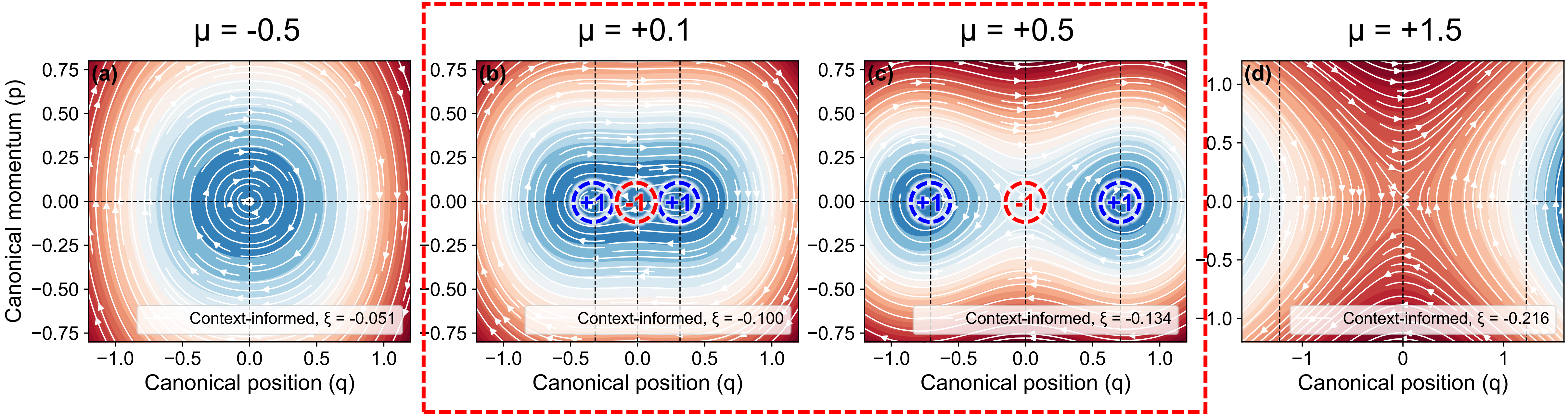

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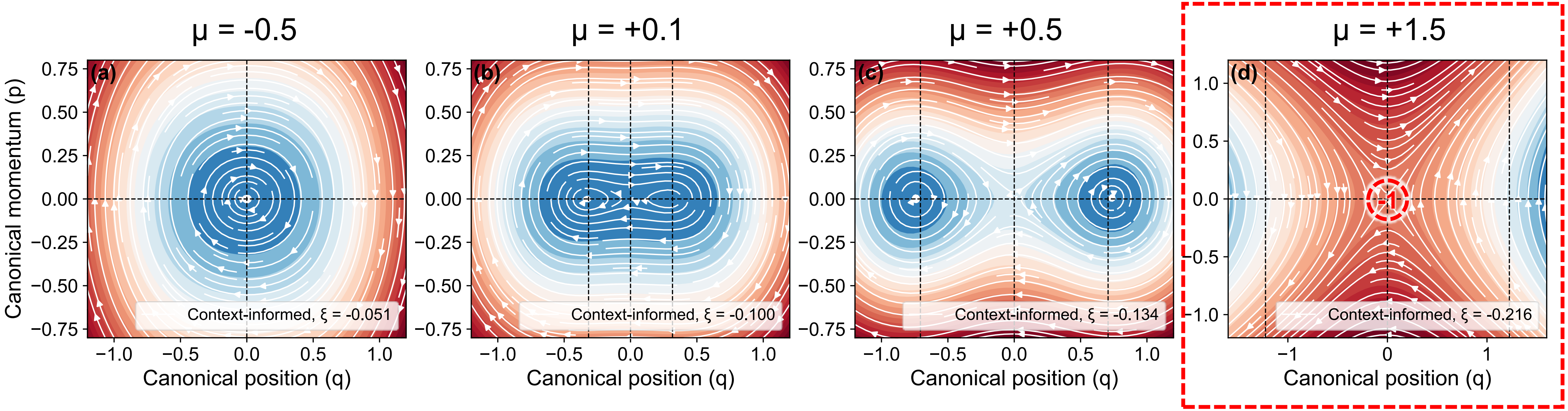
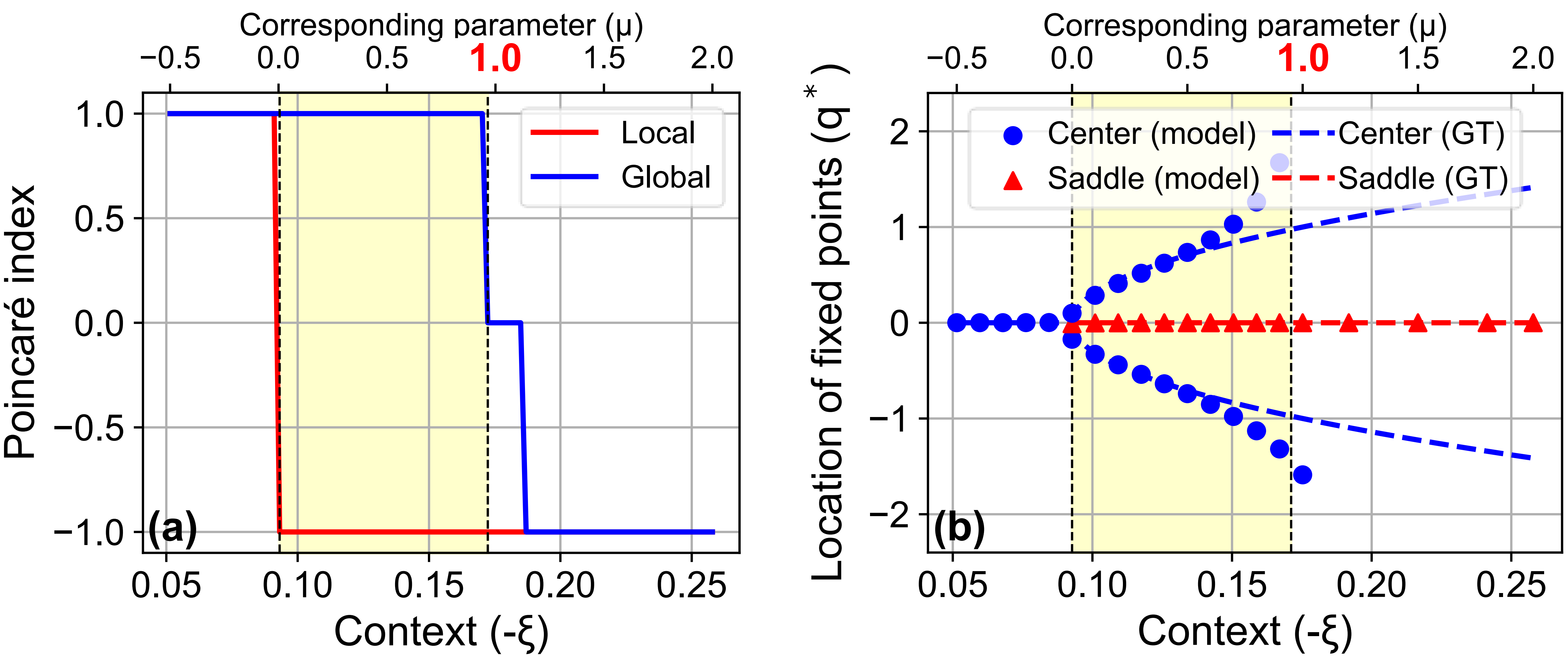
(4) As the closed orbit structure collapses for μ > 1.0, the Poincaré–Hopf theorem no longer applies, and the system simplifies into a single saddle mode.



# Insights from the Poincaré–Hopf theorem

- The global Poincaré index reliably predicts the lifetime of the correct bifurcating behaviors.



# Topology-Informed Machine Learning (TIML) via index matching

- Global topology plays a crucial role in predicting bifurcations and broken symmetries.
- Instead of letting the model learn it implicitly, why not regularize the global index explicitly?

$$\mathcal{R}_{\mathrm{PH}}(\theta_c, W, \xi_e) = \|\mathrm{Ind}(f(\cdot;\theta_c + W\xi_e), \Gamma_{\mathrm{PH}}) - \chi_{\mathrm{PH}}\|_2^2$$

Model's global index

Desired global index

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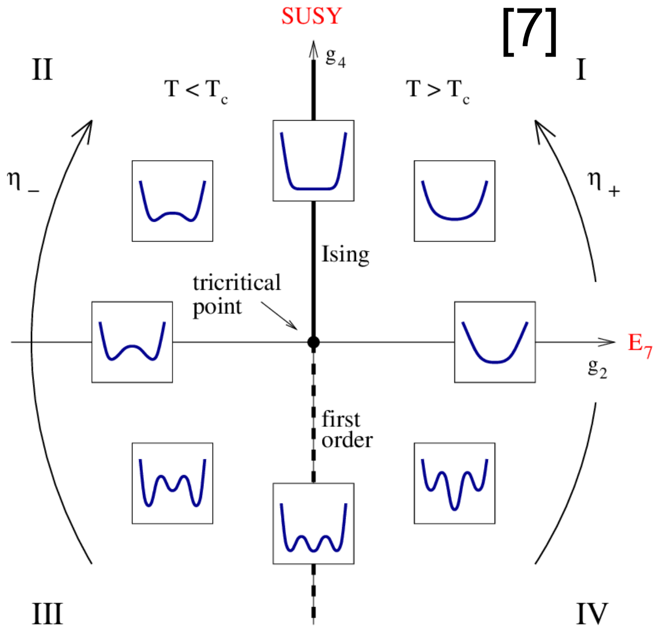
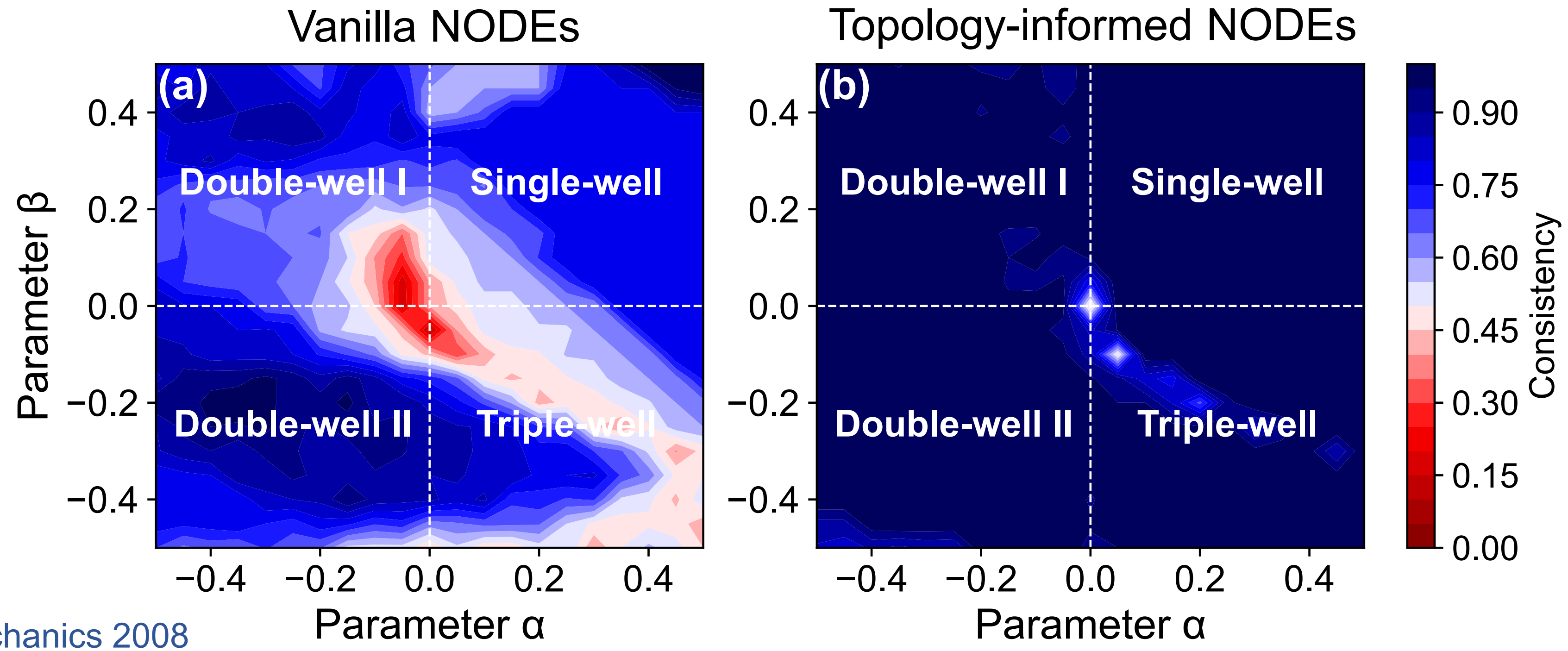
Model's global index — Desired global index

- Evaluations on complex Landau–Khalatnikov systems (used for modeling ferroelectric materials):




[7] Lepori, L. et al. Journal of Statistical Mechanics 2008

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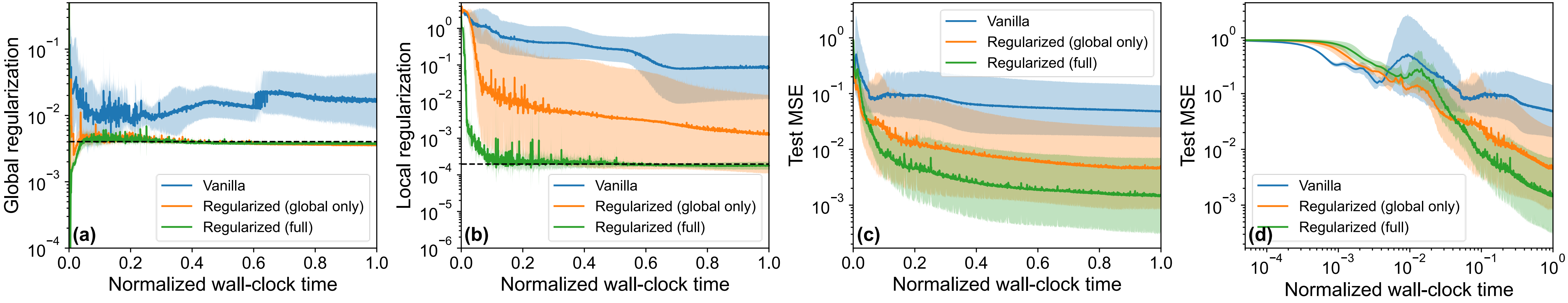


*Topology-informed ML leads to faster convergence and better predictive accuracy!*

# For more details

- In our paper, we provide:

**(1)** **Exhaustive experiments** with CI-NODEs **for identifying bifurcations** under various conditions

(2) A telling example of **hallucinated bifurcation, where the model misreads the topological structure, producing a spurious double-well** and falsely broken symmetry

**(3)** **A formal explanation** and application **of the Poincaré–Hopf theorem** to interpret results

**(4)** **Identification of cusp bifurcation**, a representative example in catastrophe theory

(5) A detailed description of **the proposed TIML framework**, including **its application to the LK system** and ablation studies