International Symposium on Lattice Field Theory 2024

Designing weight regularizations based on Lefschetz thimbles to stabilize complex Langevin

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Paul Hotzy, 29.07.2024

Content & motivation

1. Introduction: Complex Langevin & Lefschetz thimbles

2. Cosine model: A toy model where CL fails
   - Explicit check of the criterion of correctness
   - Weight regularizations: a cure for the wrong convergence

3. Reduced Polyakov loop model
   - Thimble structure depends on the coupling

4. SU(N) Polyakov loop model
   - Extending regularization ideas to SU(N) gauge theory

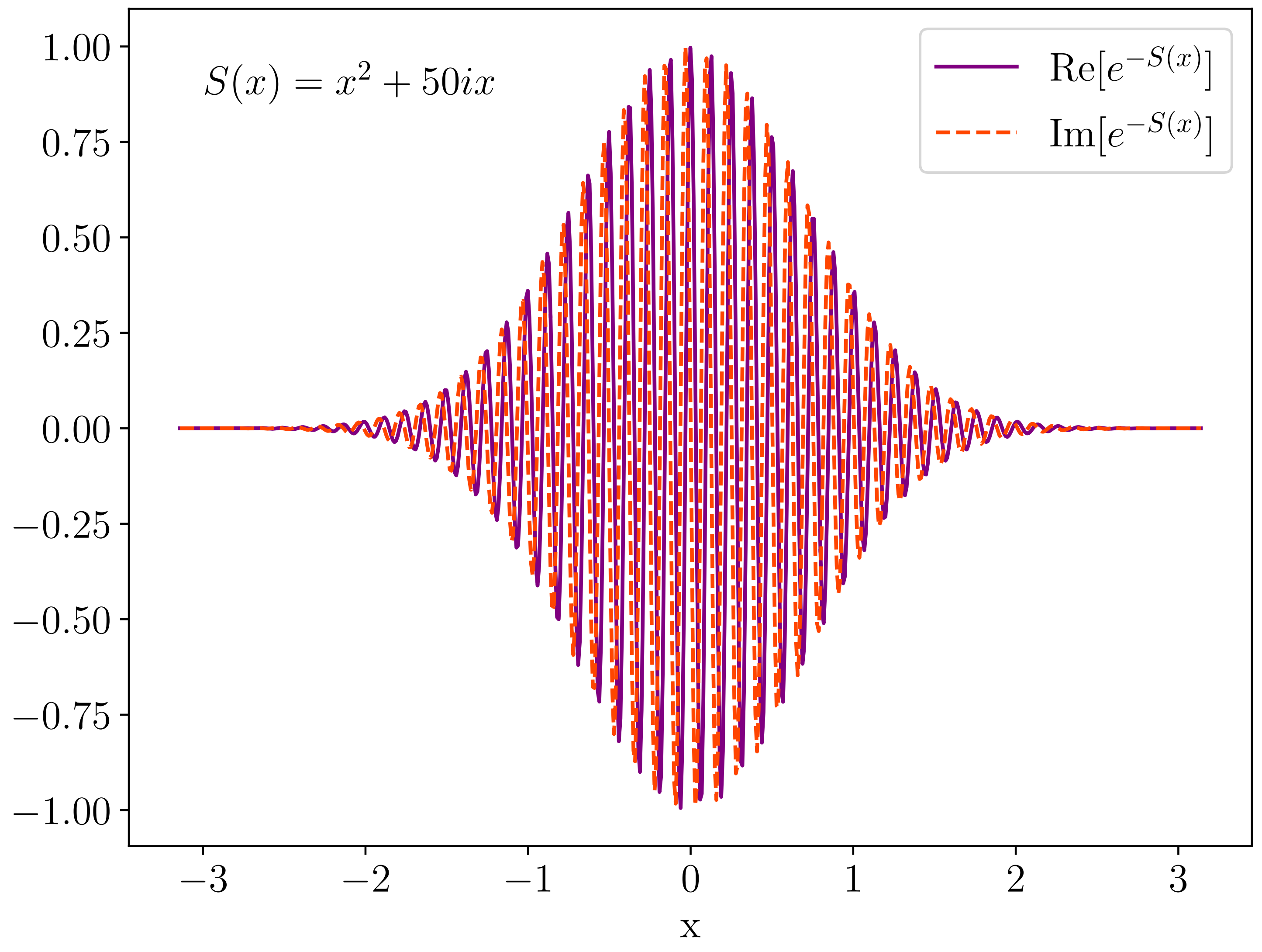
5. Outlook and conclusion

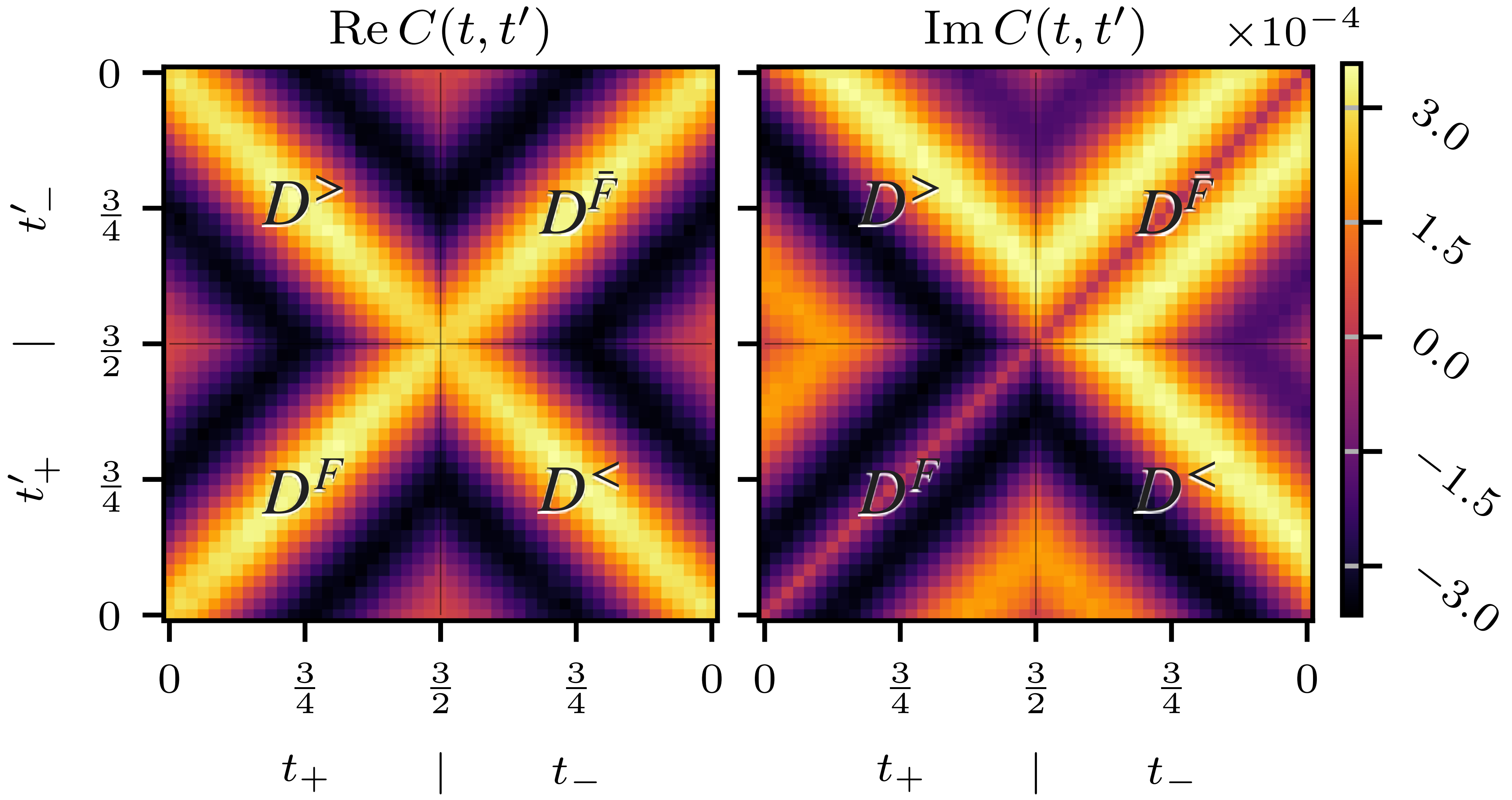
Introduction to the **complex Langevin method** and **Lefschetz thimbles**

What we are trying to achieve?

Computing… the non-deterministic polynomial hard way…

- **Expectation values:** $\langle \mathcal{O} \rangle = \frac{1}{Z}\int dx\, e^{-S(x)}\mathcal{O}(x), \quad Z = \int dx\, e^{-S(x)}$
- If S is *real*, $e^{-S(x)}/Z$ is a probability density $\rightarrow$ Monte Carlo
- If S is *complex* this does not apply $\rightarrow$ **Sign problem**





We achieved the **first results in real-time Yang-Mills results in 1+3D** (see arXiv:2312.03063)

… at small bare couplings …

$\rightarrow$ extension likely needs more work to be comp. feasible

Introduction to complex Langevin (1/2)

A naive generalization of real Langevin

- **Langevin equation**: $$\partial_\theta x(\theta) = K(x(\theta)) + \eta(\theta)$$

  auxiliary time θ

  - Drift term: $K(z(\theta)) = -S'(z(\theta))$ — describes classical evolution
  - Gaussian noise: $\eta(\theta)$ — encodes the quantum fluctuations
- **Real action S:** fields A are characterized by the limiting probability density $P(\theta \to \infty) \propto e^{-S}$
- **Complex action S:** drift term is complex — we need to complexify the dyn. variables $x \to z = x + iy$

Introduction to complex Langevin (2/2)

A *less* naive generalization of real Langevin

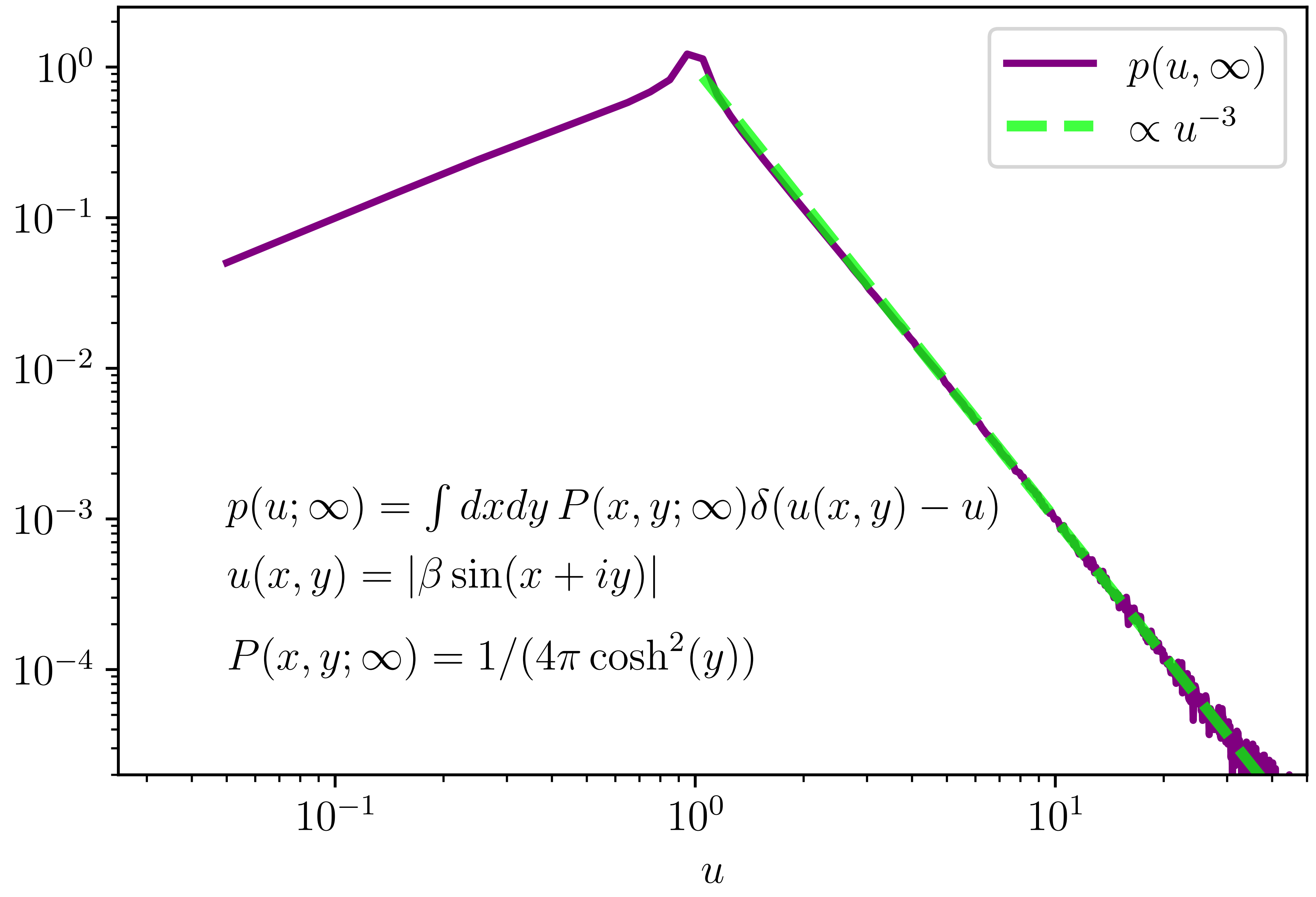
- **Expectation values with complex Langevin:**

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int_D dx \exp[-S(x)] \mathcal{O}(x) = \lim_{\Theta \to \infty} \int_{\theta_0}^{\theta_0 + \Theta} d\theta \mathcal{O}(z(\theta))$$

- Correspondence to Fokker-Planck equation: $\partial_\theta P(x, y; \theta) = L^T P, \quad L^T = \partial_x(\partial_x + \mathrm{Re}K) + \partial_y \mathrm{Im}K$

- **Criterion of correctness** — we know when it fails:
  - Density of drift magnitude has to decay exponetially

$$p(u; \theta) = \int dx \int dy \, \delta(u - u(z)) P(x, y; \theta), \; u(z) = |K(z)|$$



- **But what shall we do if the criterion is not satisfied?**

Lefschetz thimble approach

Application of the Cauchys theorem to the path integral

- Complexify the dynamical variables: $x \to z = x + iy$

$$Z = \int_D dz\, \exp(-S(z)) = \sum_\sigma n_\sigma e^{-i\mathrm{Im}[S(z_\sigma)]} \int_{D_\sigma} dz\, e^{-\mathrm{Re}[S(z)]} =: \sum_\sigma n_\sigma e^{-i\mathrm{Im}[S(z_\sigma)]} Z_\sigma$$

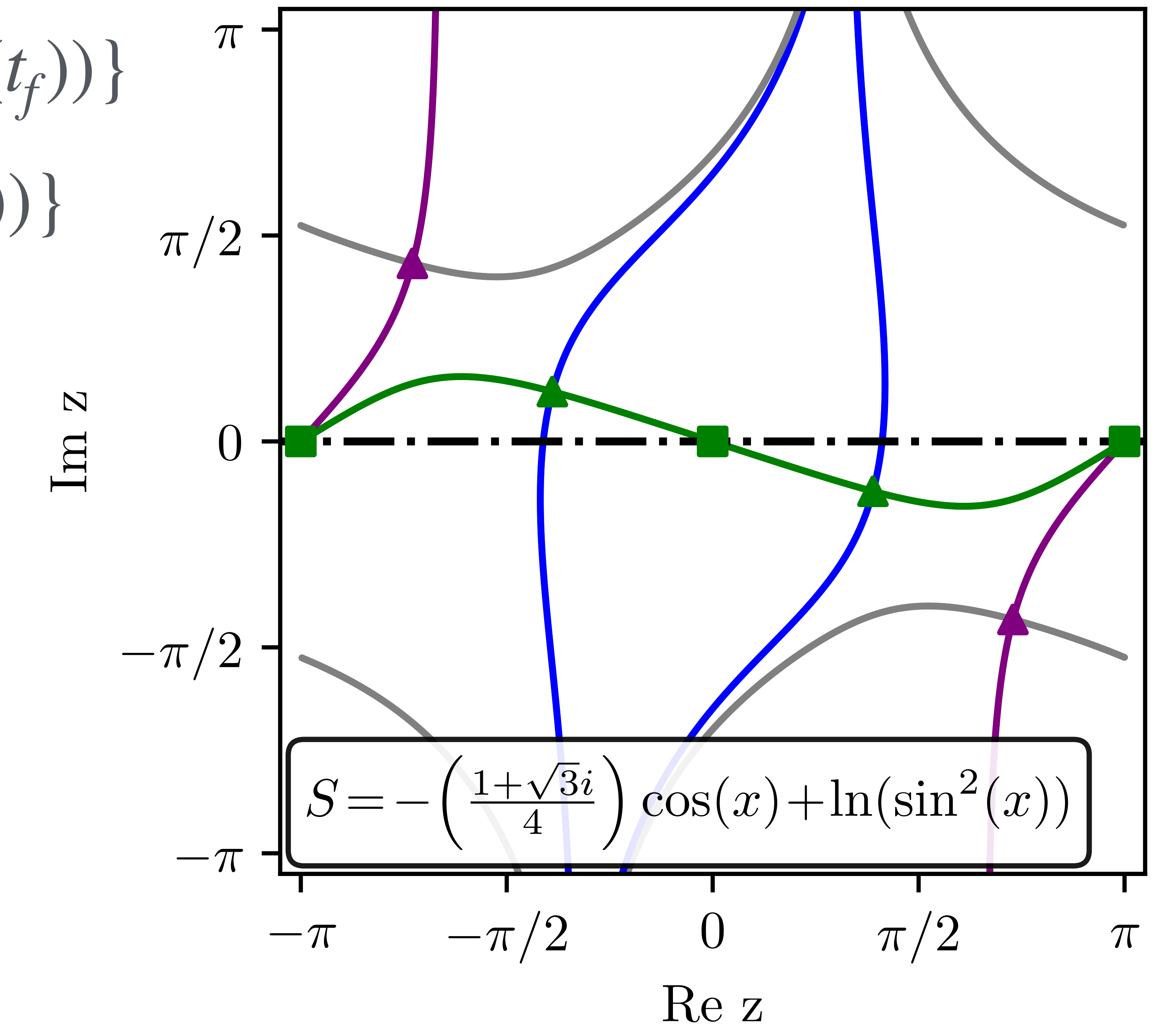
(n_σ number of intersections of K_σ and D, z_σ are stationary points of the action S)

- Thimbles (SD paths): $D_\sigma := \{z(t_f) \in \mathbb{C} : z(-\infty) = z_\sigma, \dot{z}(t_f) = -\overline{S}'(z(t_f))\}$
- Co-thimbles (SA paths): $K_\sigma := \{z(t_f) \in \mathbb{C} : z(-\infty) = z_\sigma, \dot{z}(t_f) = \overline{S}'(z(t_f))\}$

- **Expectation values with Lefschetz thimbles:**

$$\langle \mathcal{O} \rangle = \frac{\sum_\sigma n_\sigma e^{-i\mathrm{Im}[S(z_\sigma)]} Z_\sigma \langle \mathcal{O} \rangle_{Z_\sigma}}{\sum_\sigma n_\sigma e^{-i\mathrm{Im}[S(z_\sigma)]} Z_\sigma}$$

Monte Carlo feasible!

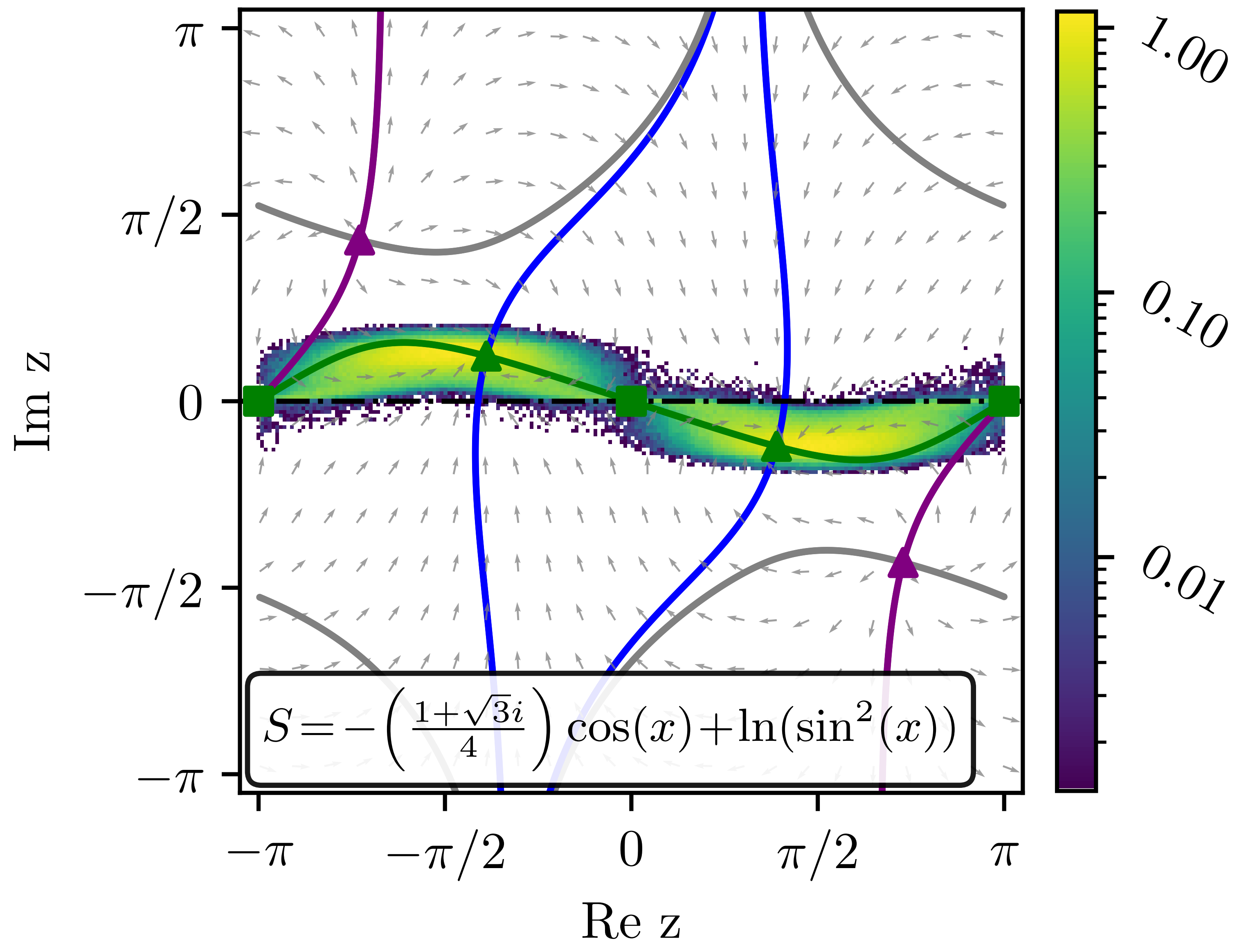


Nothing but intuition and a hunch…

Connection between Lefschetz thimbles and complex Langevin

Similarities between CL and LT:

1. Analytical continuation of theories
2. Introduction of auxiliary times θ and t_f
3. CL drift term $-S'$ and flow equation $-\overline{S}'$



Complex Langevin is sometimes considered to be an "*important sampling near to thimbles*"

→ rather an important sampling near attractive stationary points

- Connection is not well understood — is the criterion of correctness for CL linked to LT?
- ***We use the Lefschetz thimble as a tool to regularize for complex Langevin!***

Total failure of complex Langevin:
Complex cosine model

Complex cosine model

Non-trivial but fully controlled model with wrong convergence of CL

- **Weight function** of complex cosine model:

$$\rho(x) = e^{-i\beta\cos(x)},\ \beta \in \mathbb{R}$$

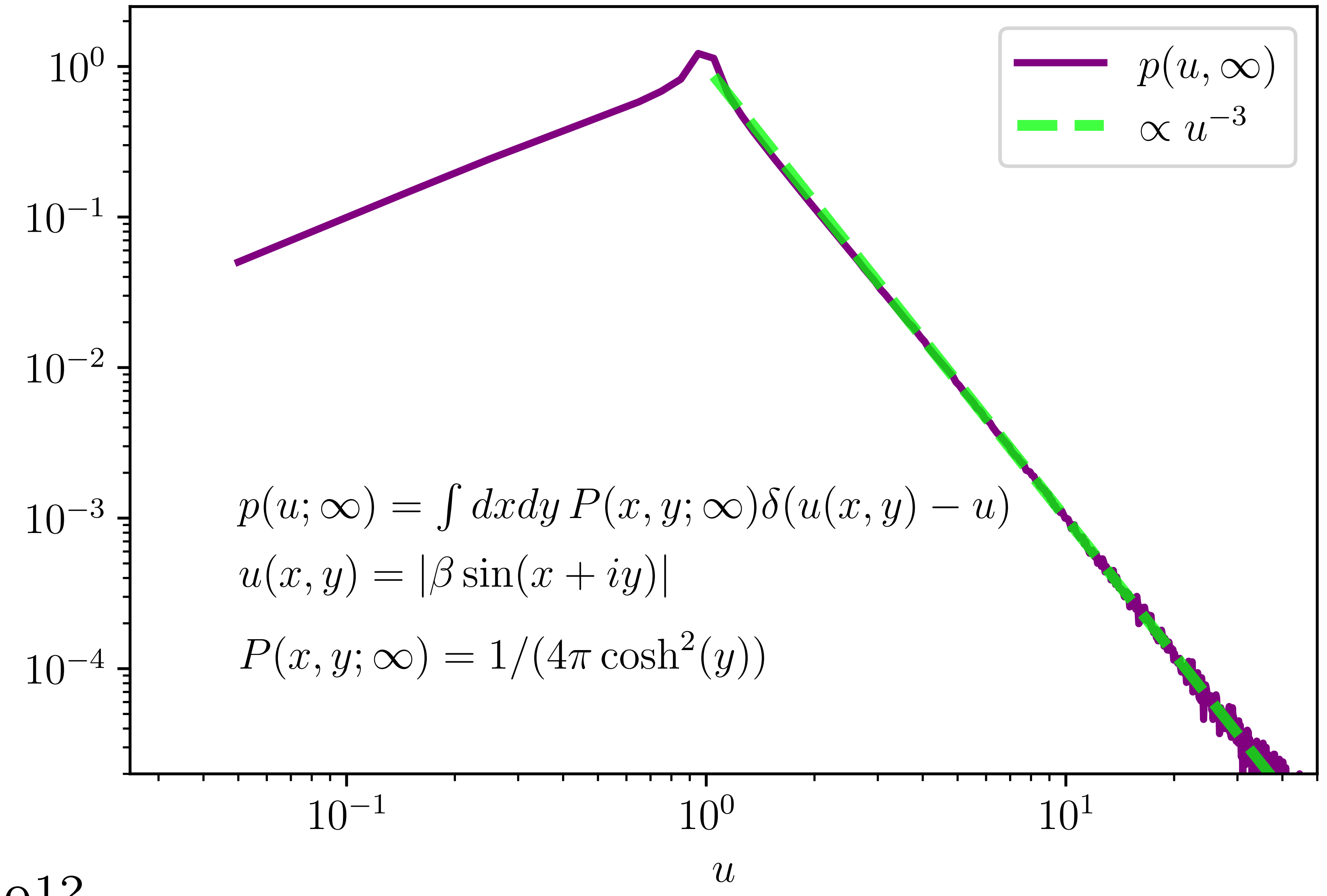
- **Stationary solution** of the stochastic process:

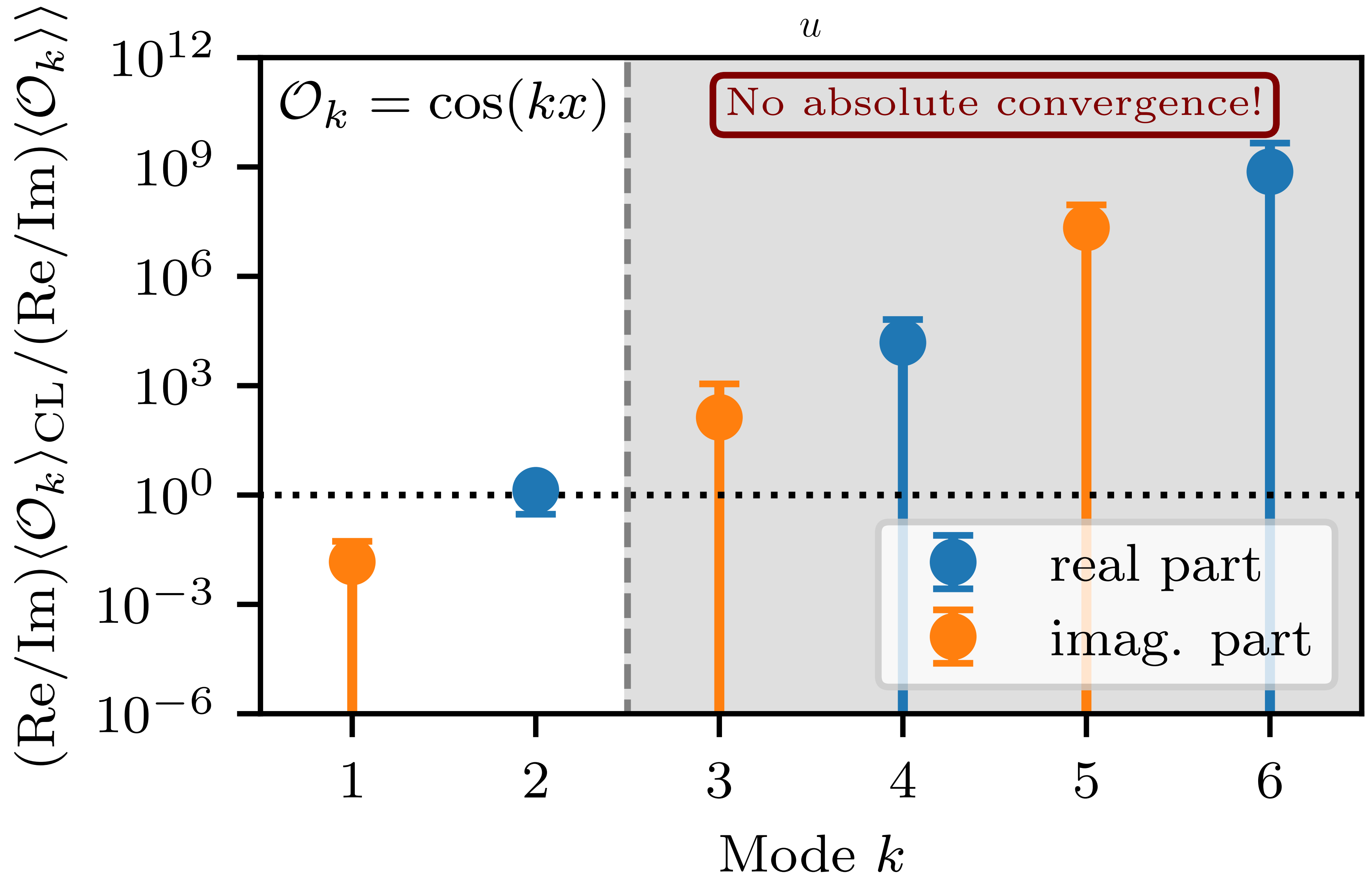
$$P_{\mathrm{st}}(x,y) = \frac{1}{4\pi\cosh^2(y)}$$

- **Criterion of correctness is not satisfied:**
  - Emergence of boundary terms [arXiv:1808.05187]
  - Decay of density of drift magnitude (right figure)

- Analytic expectation values (bottom figure):

$$\langle \mathcal{O}_k \rangle = \int_{[-\pi,\pi]} dx\, \rho(x)\cos(kx) = (-1)^k \frac{J_k(\beta)}{J_0(\beta)}$$





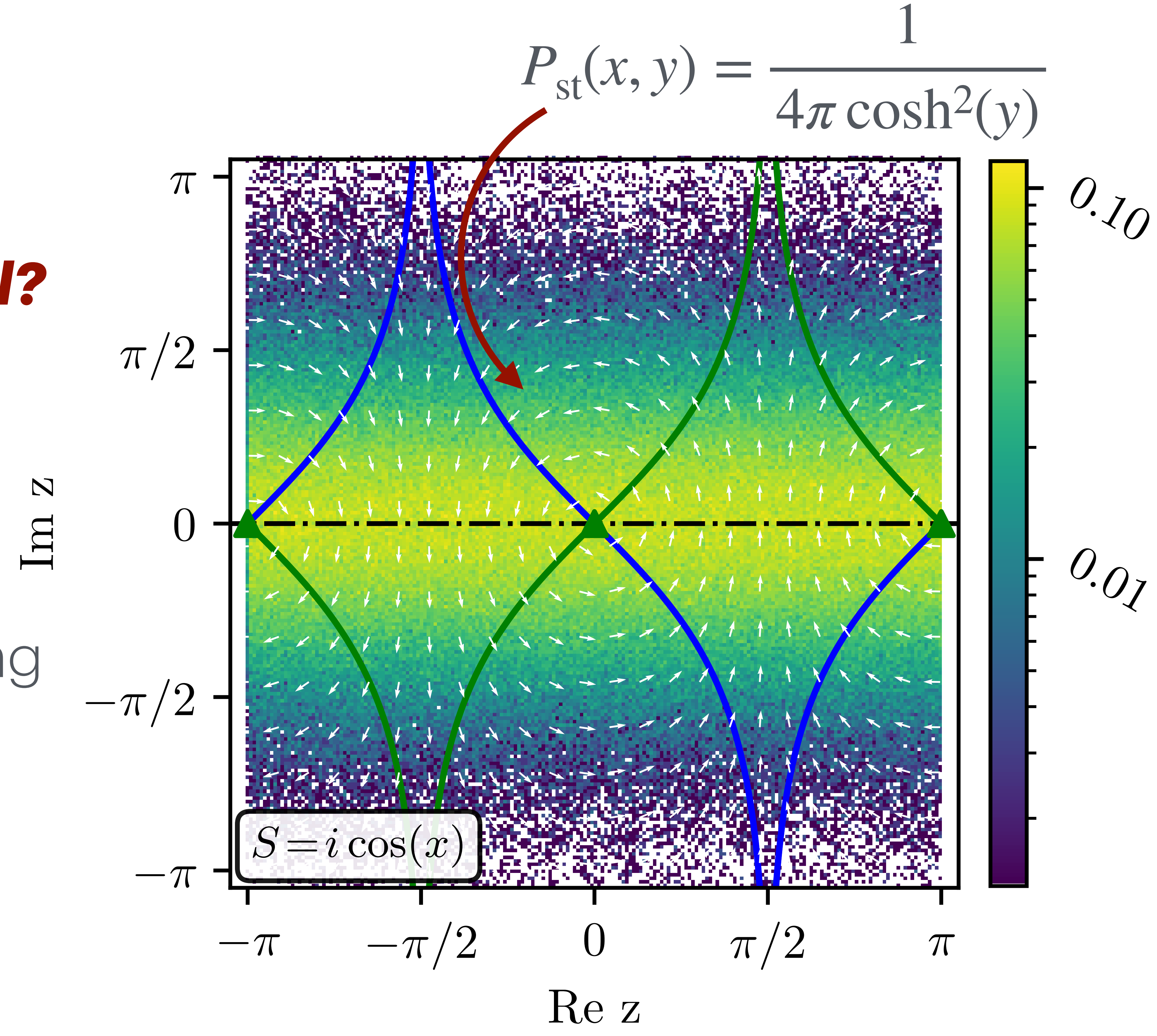
Thimbles of the cosine model

Simple structure with obvious consequences

- Established "criterions of correctness" or **mostly diagnostic**
  - Decay of drift magnitude
  - Boundary terms

What should we do if they fail?

- Lefschetz thimbles might allow for a more detailed understanding of the Langevin dynamics:
  - Attractive/repulsive stationary points and singularities
  - Weights and probability currents



Designing weight regularizations

If you cannot simulate the theory — change the theory

- Add a **regularization term** to the original weight

$$\rho(x) \quad \rightsquigarrow \quad \rho_R(x) := \rho(x) + R(x)$$

- We modify/"regularize" the weight with three objectives

1. **Stationary points** should be **close to the real line**
2. **Singularities** that connect to contributing thimbles should be **on the real line**
3. We want to **avoid any asymptotic structure** of contributing thimbles ("tamed" thimbles)

Similiar ideas have been investigated before:
Z. Cai et al arXiv:2109.12762
F. Attanasio et al arXiv:1808.04400
A. C. Loheac et al arXiv:1702.04666
S. Tsutsui et al arXiv:1508.04231
…

In general those objectives are not achievable for neutral regularization — **expectation values change and we need to compute corrections!**

Curing the criterion of correctness

Regularization cures the wrong convergence issue

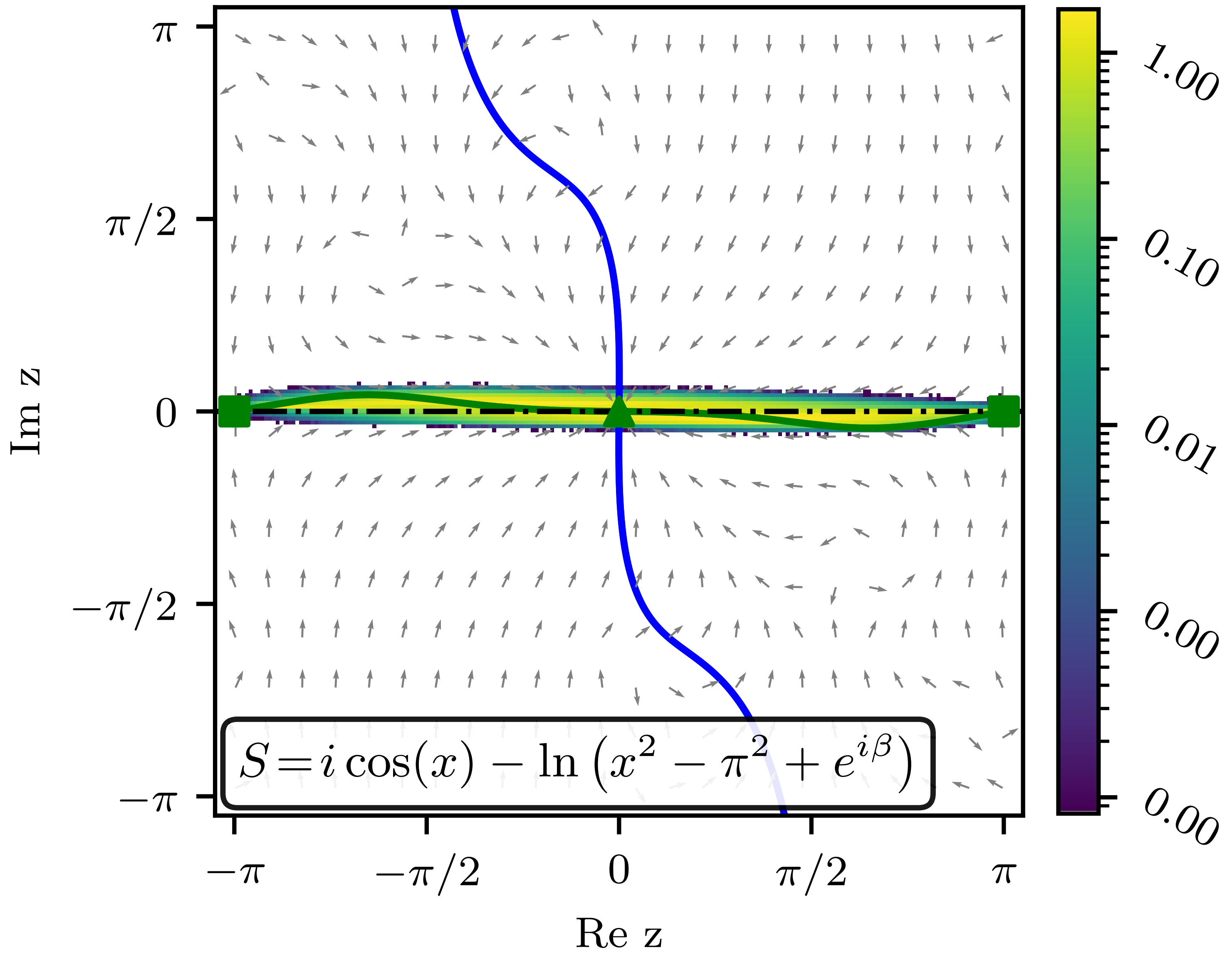
- **Regularization of the cosine model**

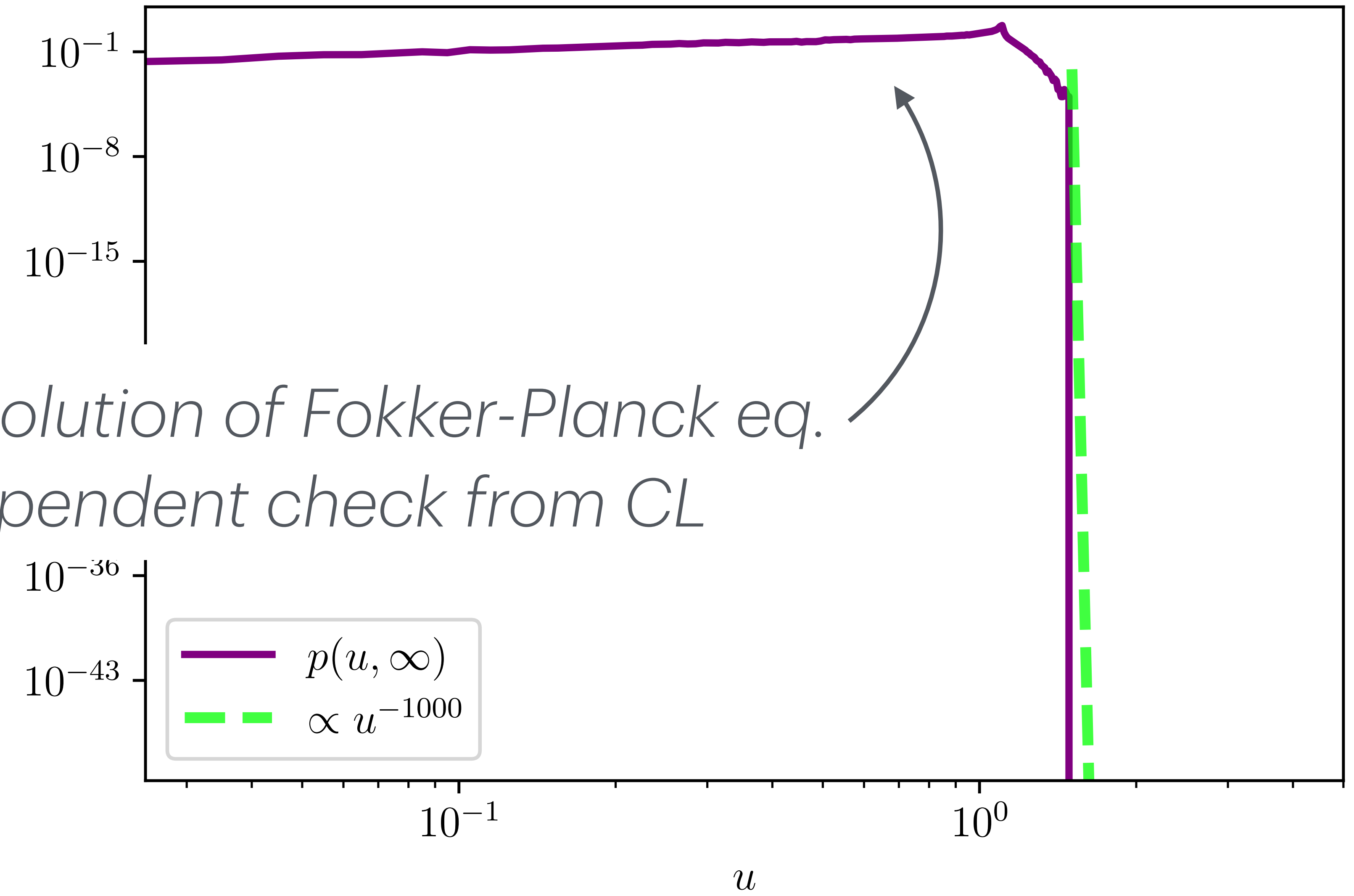
$$\rho_R(x) = e^{i\beta\cos(x)} + R(x)$$

$$R(x) = r(x^2 - \pi^2) - \exp(i\beta), r \in \mathbb{C}$$

- **Regularization term achieves our goals:**
  1. Polynomial term leads to one stationary point at the origin
  2. Constant shifts singularities to the $\pm\pi$
  3. No asymptotic structure of thimbles, for $|r| \to \infty$ we have the drift:

$$\text{Im}\left[K_R(x+iy)\right] = -y\left[\frac{1}{(x-\pi)^2+y^2} + \frac{1}{(x+\pi)^2+y^2}\right]$$





Direct solution of Fokker-Planck eq.
— independent check from CL

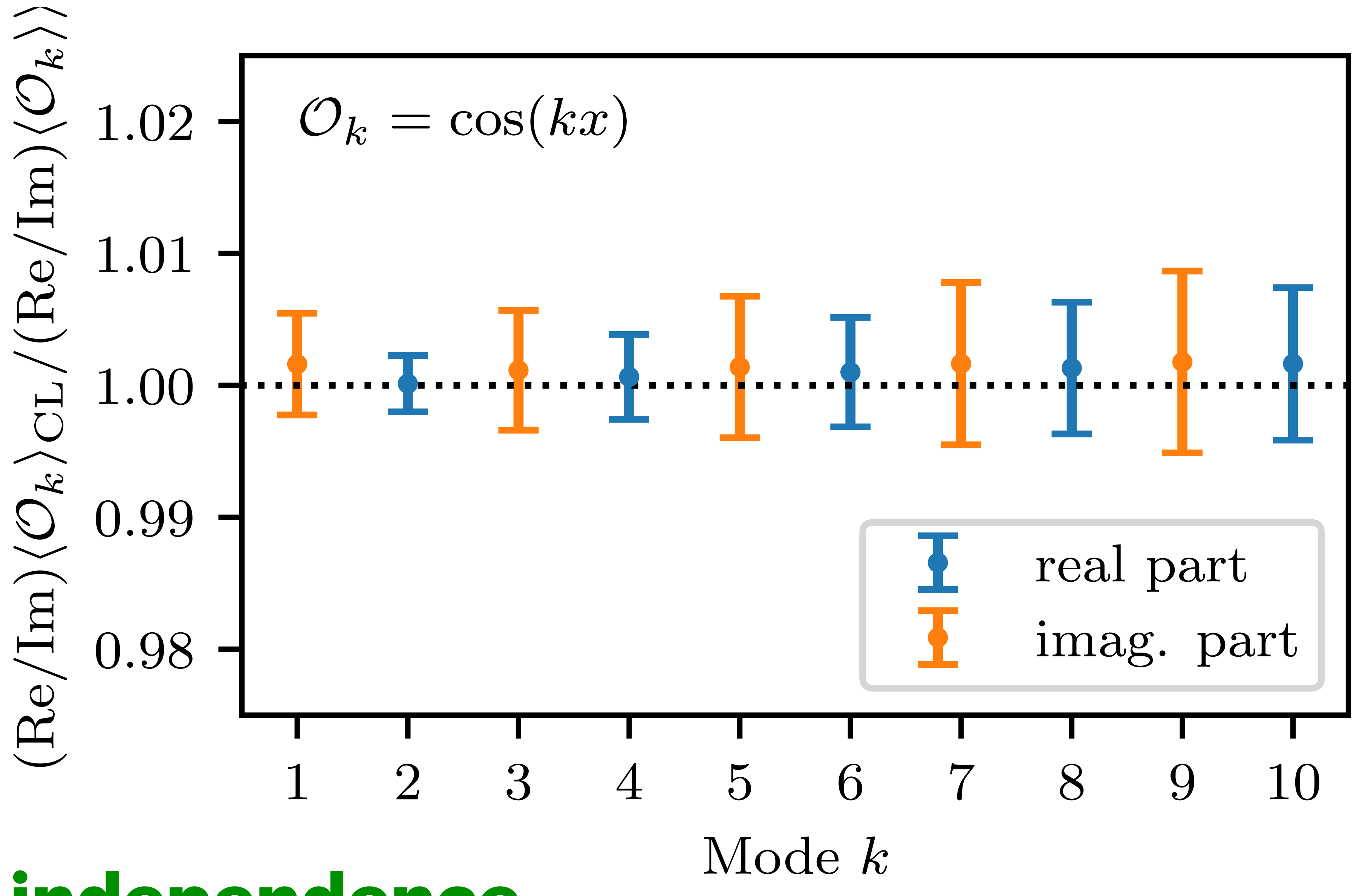
Corrections for regularizations

Apriori knowledge allows computation of correction term

- **Correction term** for regularized expectation values

$$\langle \mathcal{O} \rangle_\rho = \langle \mathcal{O} \rangle_{\rho_R} + \mathrm{Corr}_R(\mathcal{O})$$

$$\mathrm{Corr}_R(\mathcal{O}) = (\langle \mathcal{O} \rangle_{\rho_R} + \langle \mathcal{O} \rangle_R) Q, \quad Q = \frac{Z_R}{Z_\rho}$$



- How to compute **the bad guy Q?**

→ Apriori knowledge of the original system — observable independence

Vanishes for $r \to \infty$!

Dyson-Schwinger equation: $\langle \mathcal{O}^* \rangle_\rho = \langle \mathcal{O}' - \mathcal{O}S' \rangle_\rho = 0 \;\rightarrow\; Q = \dfrac{\langle \mathcal{O}^* \rangle_{\rho_R}}{\langle \mathcal{O}^* \rangle_R - \langle \mathcal{O}^* \rangle_{\rho_R}}$

Option for the cosine model: $\mathcal{O}^* = \cos(x) + i\beta \sin(x)\cos(x)$

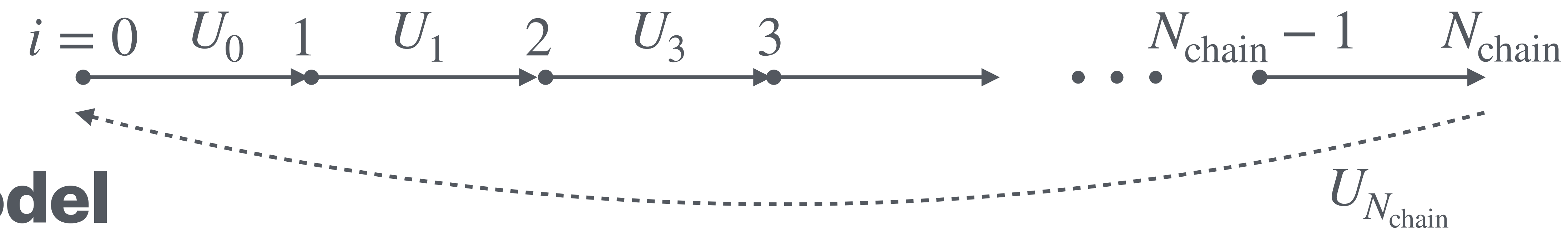
A model where CL fails, depending on the coupling:

Polyakov loop model

Reduced Polyakov loop model (1/2)

Reducing a gauge theory to a scalar theory

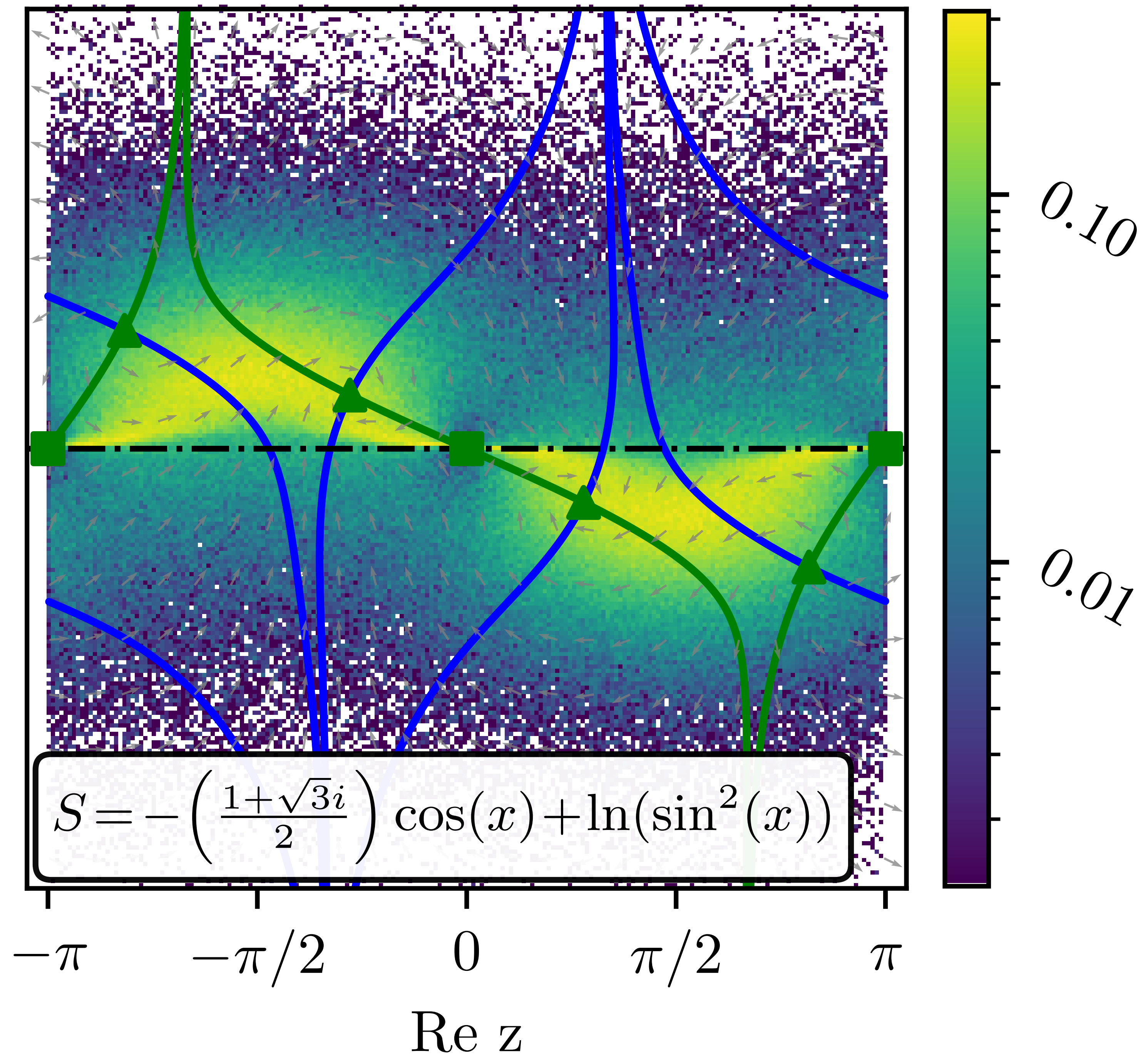
$$P = \prod_{i=0}^{N_{\text{chain}}} U_i, \quad U_i \in \mathrm{SU}(N_c)$$



- **Polyakov loop action** in SU(2) (*SU(3) is in progress*):

$$S = -\beta \mathrm{Tr}(P),\ \beta \in \mathbb{C}$$

- Gauge freedom leads to equivalence to the **one-link model**
- **Reduction of the Haar measure**
  - $\displaystyle\int_{SU(2)} dU\, e^{\beta \mathrm{Tr}(U)} \rightsquigarrow \int_{-\pi}^{\pi} dx\ \sin^2(x) e^{2\beta\cos(x)}$
- **Identify observables and (scalar) effective action**
  - $S(x) = -2\beta\cos(x) - \ln(\sin(x)^2), \quad \mathrm{Tr}(U) \leftrightarrow 2\cos(x)$

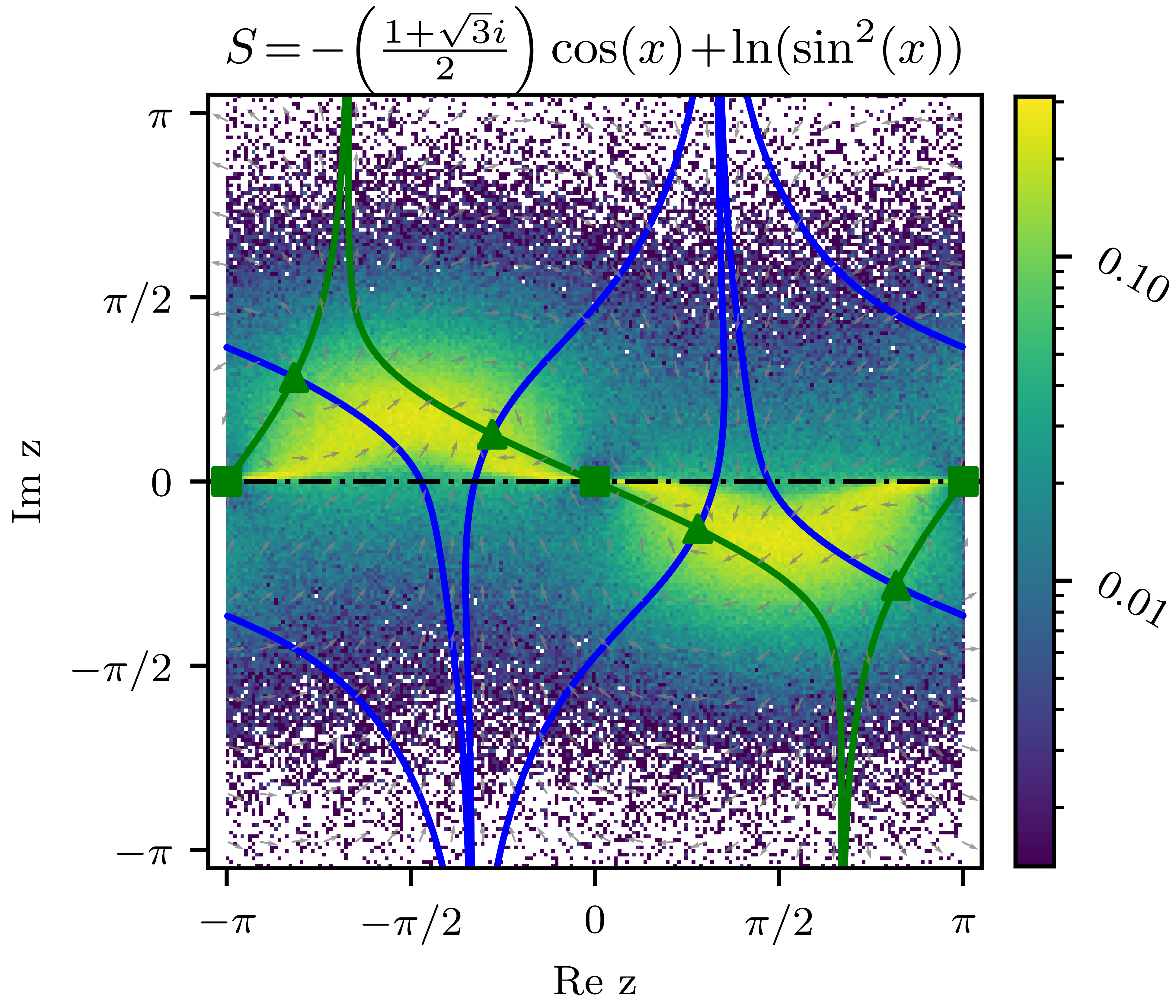


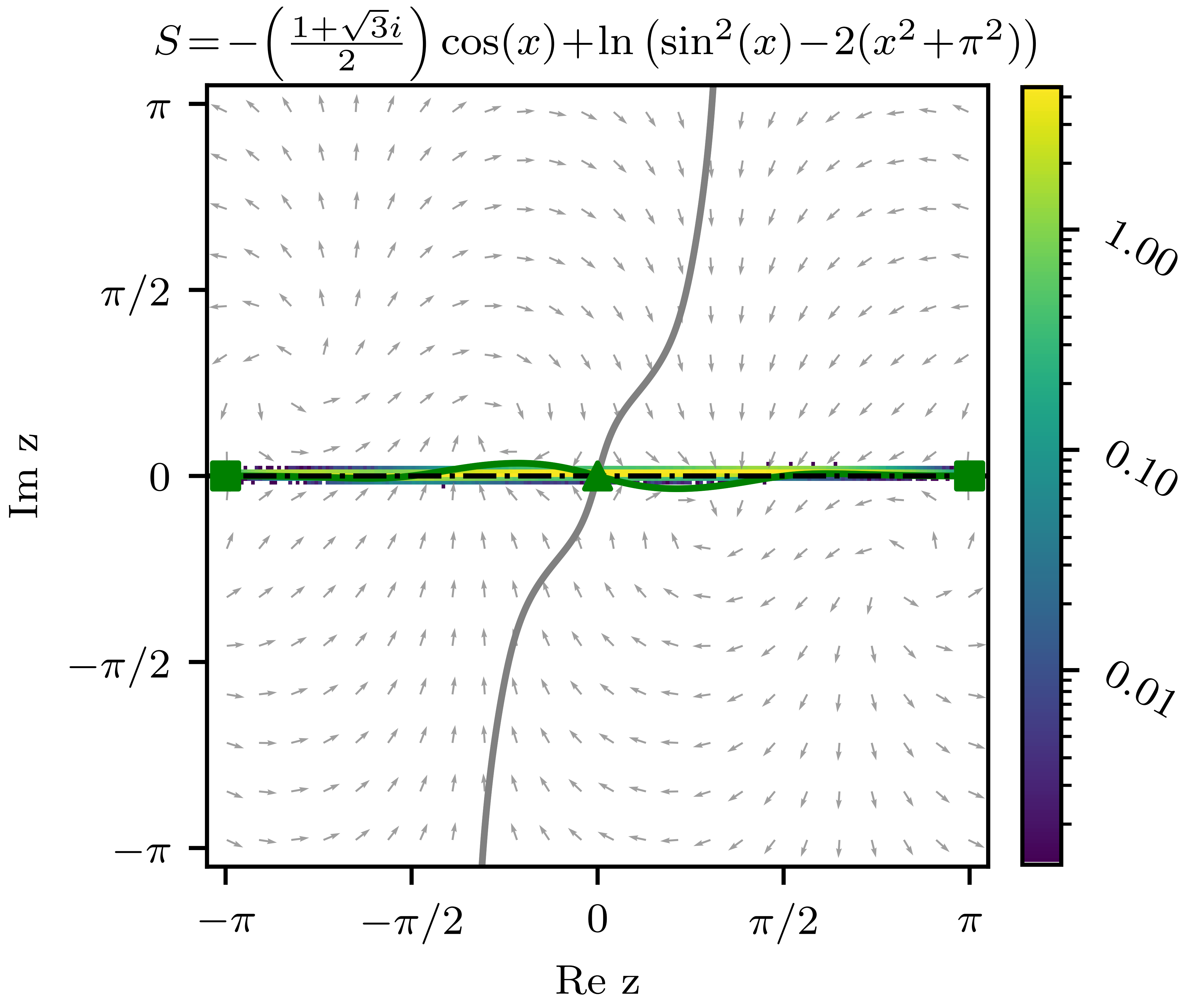
Reduced Polyakov loop model (2/2)

Regulazing the reduced Polyakov — different model, same idea

The same ideas as for the cosine model apply:

$$\rho(x) = \exp[2\beta\cos(x) + \ln(\sin(x)^2)] \rightsquigarrow \rho_R(x) = \rho(x) + R(x) = \rho(x) + r(x^2 - \pi^2)$$





Polyakov loop model (1/2)

Can we generalize these regularizations to SU(N) gauge theories?

- **Action of the Polyakov loop model:** $S[\{U_i\}] = -\beta \mathrm{Tr}\left[\prod_i U_i\right]$
- SU(N) is compact, for SU(2) the trace of the links is bounded: $\mathrm{Tr}[U] \in [-2,2]$
- **The first thing that comes to mind …**

$$\rho[\{U_i\}] = \exp[\beta \mathrm{Tr}[P]] \rightsquigarrow \rho_R[\{U_i\}] = \rho[\{U_i\}] + R[\{U_i\}] = \rho(x) + r\left\{(\mathrm{Tr}[P]/N_c)^2 - 1\right\}$$

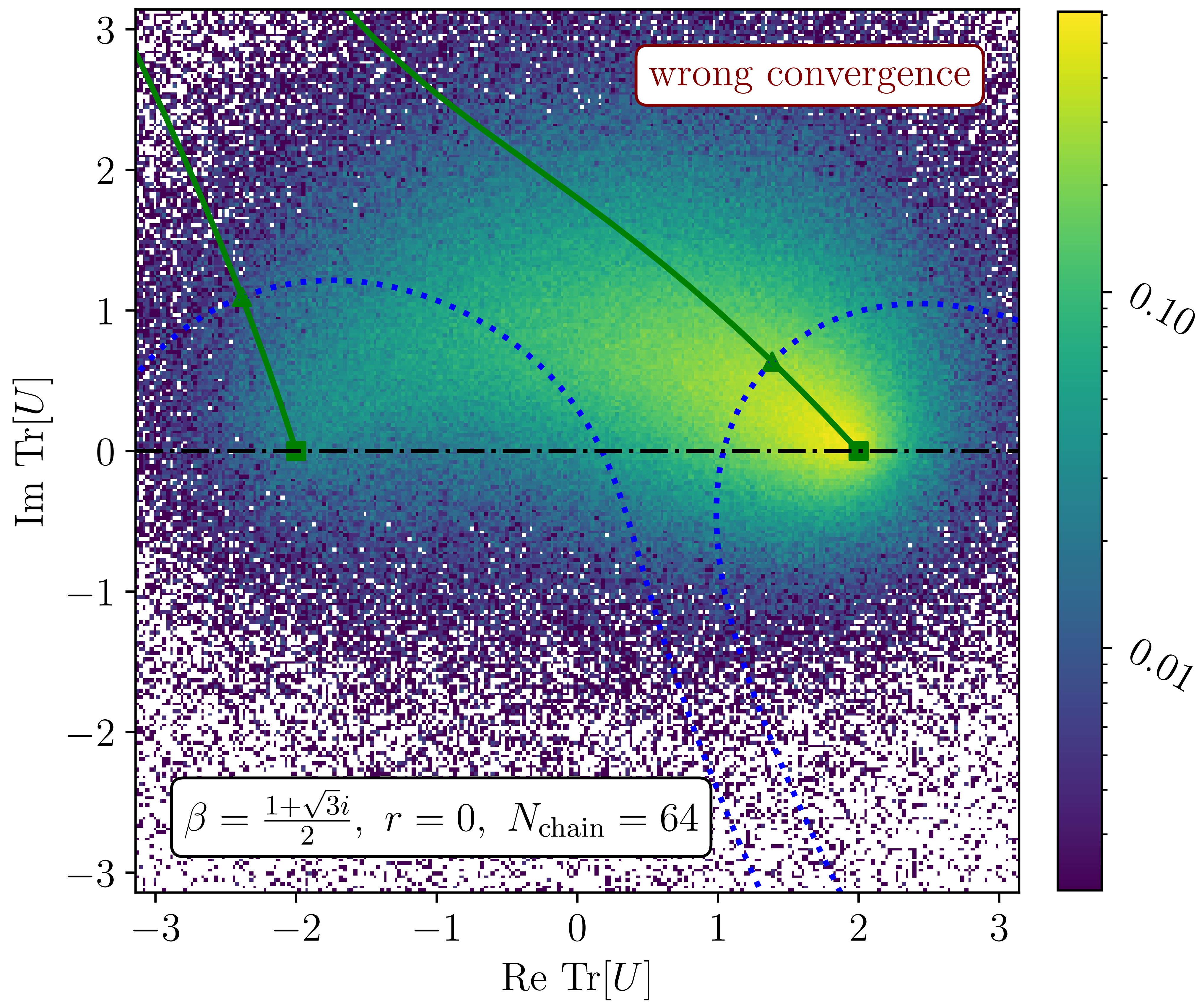
… and it works.

- Sidenote: $\mathrm{SL}(N_c, \mathbb{C})$ is non-compact! We use the gauge cooling technique to stabilize the system — however, we observed that we do not need it for large enough r.

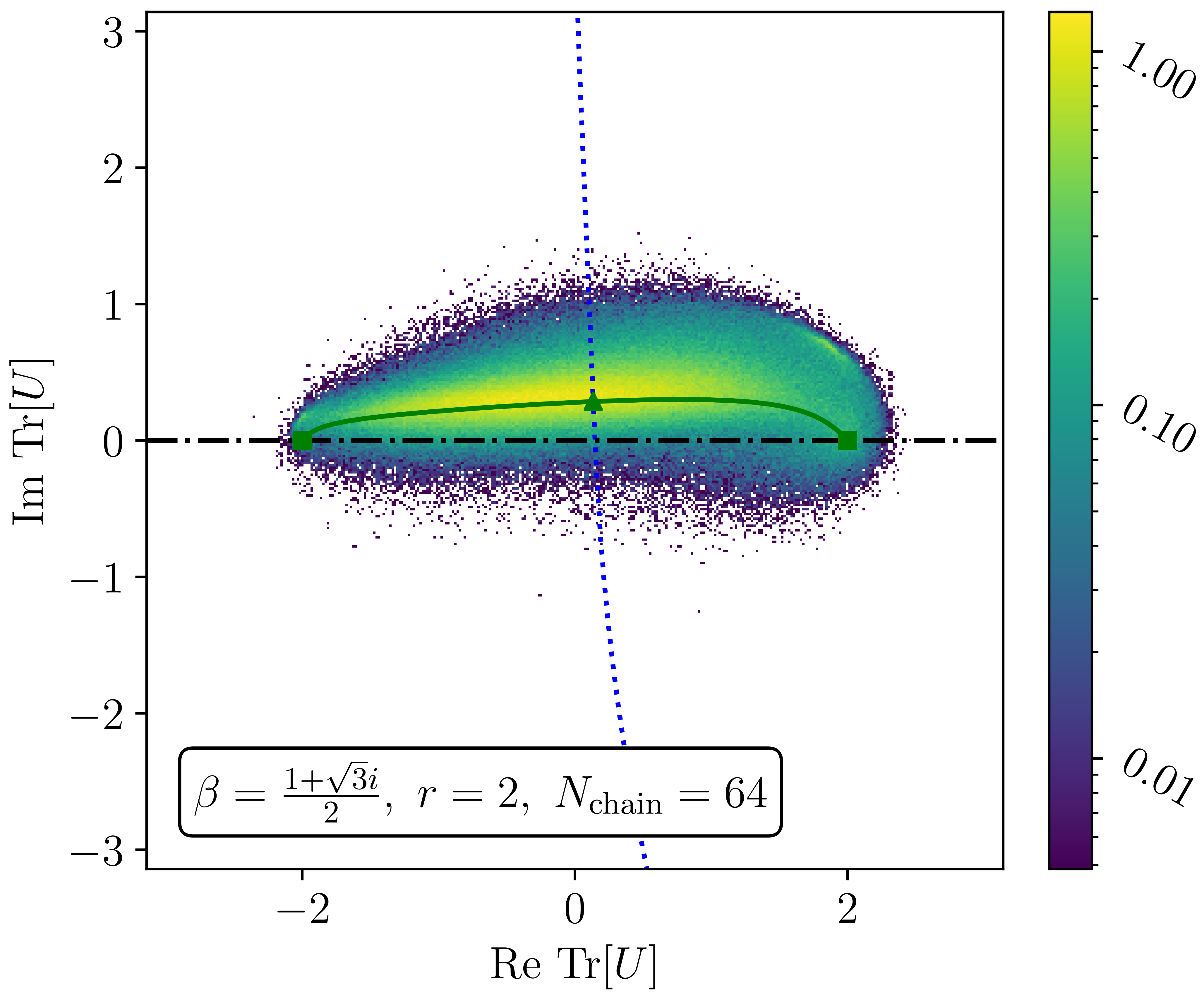
Polyakov loop model (2/2)

A first step towards lattice gauge theories

Without regularization:



With regularization:



Conclusion

- Complex Langevin often fails due to the slow decay of the drift density
- Criterion of correctness is linked to the structure of the Lefschetz thimbles
- **We cure the wrong convergence issue by regularizing the weight function:**
  - Design regularizations to obtain a **compact thimble structure**
  - We obtain **corrections from apriori knowledge** using Dyson Schwinger equations

→ Solution to the complex cosine model and the Polyakov loop model

→ Extension to lattice Yang-Mills theory is work in progress

Goal: application to real-time Yang-Mills theory

Thank you for your attention!

Extensions to actual lattice gauge theory

Locality and extensivity of the weight function and regularization

- Consider SU(N) Yang-Mills theory on an $N_s^3 \times N_t$ lattice with the Wilson action

$$\rho = \exp(-S) = \prod_x e^{-\frac{1}{g^2}\sum_{\mu\neq\nu}\rho_{\mu\nu}\mathrm{Tr}\left[U_{x,\mu\nu} - \mathbf{1}\right]} =: \prod_x \rho_x$$

- **'Global' regularization:** $\rho_R = \rho + R$ $\rightarrow$ global drift term, extensivity leads to problems

- **'Local' regularization:** $\rho_R = \prod_x (\rho_x + R_x)$ $\rightarrow$ correction procedure becomes complicated

<u>Ideas / work in progress:</u>

- We can achieve desirable thimbles structures with **multiplicative regularizations** — essentially reweighting, but with respect to a complex weights (by design no hard overlap problem).

- We develop a <u>mathematical</u> connection between thimbles and CL that allows us to **design kernel transformaltion** that admit similar Lefschetz thimbles.