SIGN25 Workshop in Bern, Switzerland

Enhancing Complex Langevin with Lefschetz Thimble-Based Regularizations

In collaboration with Kirill Boguslavski and David I. Müller

arXiv:2412.02396

Paul Hotzy, 23.01.2025

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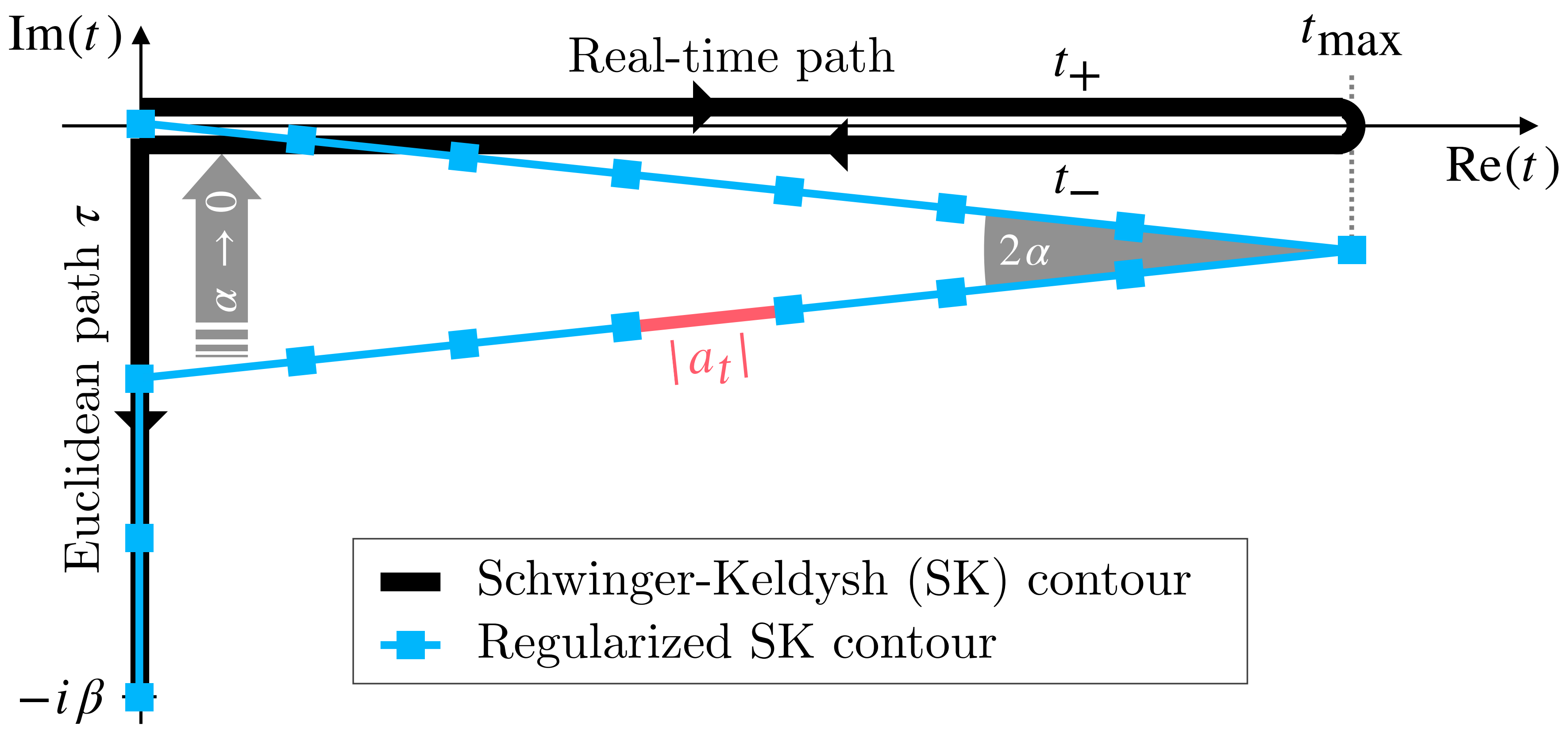
Introduction to the **complex Langevin method** and **Lefschetz thimbles**

What we are trying to achieve?

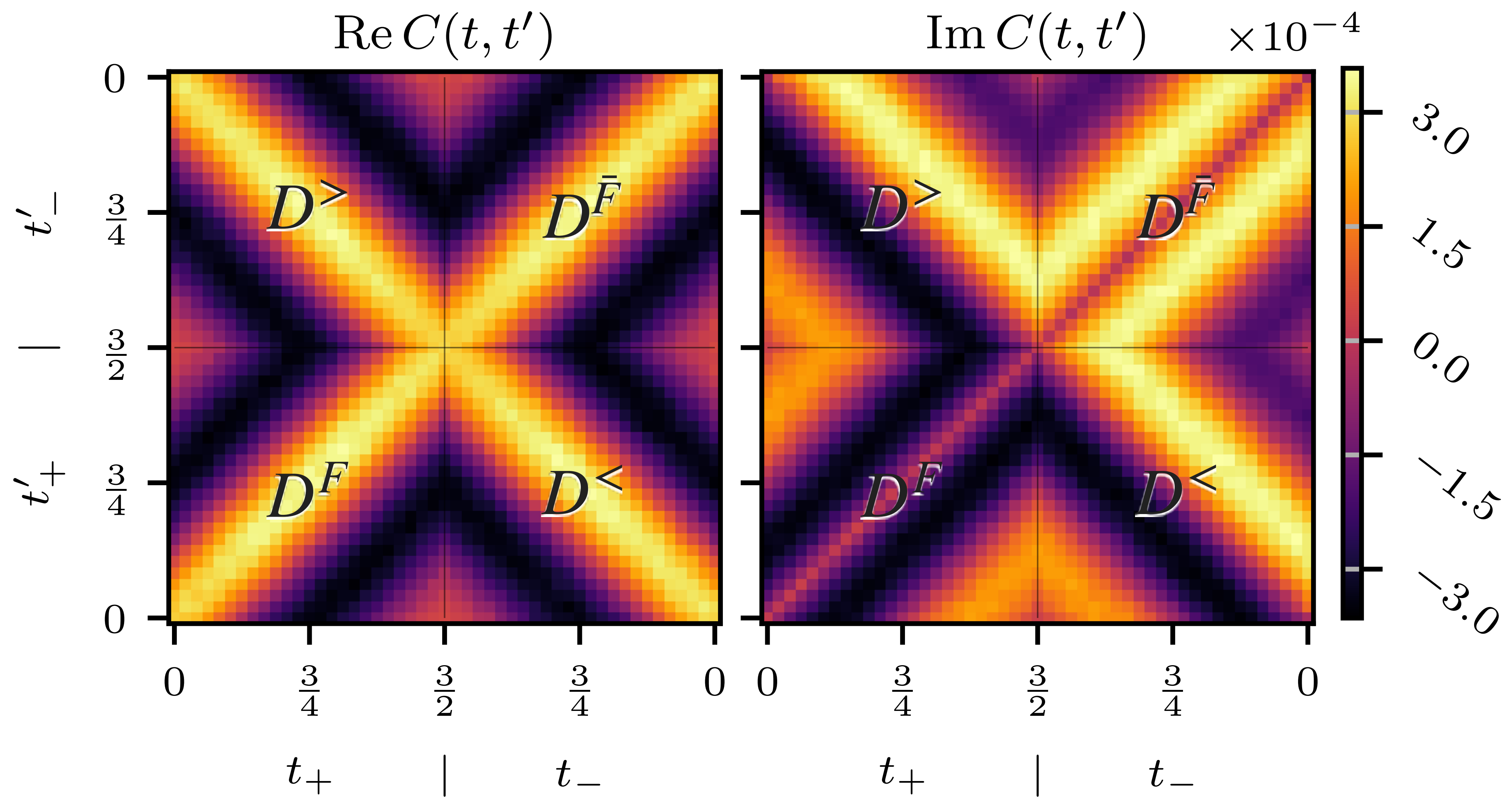
Computing… the non-deterministic polynomial hard way…

Expectation values:

$$\langle \mathcal{O}[A] \rangle = \frac{1}{Z} \int \mathcal{D}A_E \, e^{-S_E[A_E]} \int \mathcal{D}A_+ \, \mathcal{D}A_- \, e^{iS[A_+,A_-]} \, \mathcal{O}\left[A_+, A_-, A_E\right]$$



1. If S is *real*, $e^{-S(x)}/Z$ is a probability density → Monte Carlo
2. If S is *complex* this does not apply → **Sign problem**



We computed unequal real-time correlation fcts. for **Yang-Mills results in 1+3D** (see talk on Fri 11:30)
… at small bare couplings …

→ extension is work in progress

Introduction to complex Langevin (1/2)

A naive generalization of real Langevin

- **Langevin equation**: $$\partial_\theta z(\theta) = K(z(\theta)) + \eta(\theta)$$ 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:** dyn. variables x 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 $x \to z = x + iy$

✳ CL yields (provided it is stable) a real density $P(x, y) \in \mathbb{R}$, but is the one we are looking for?

$$\int dx\, \mathcal{O}(x) e^{-S(x)} = \int dxdy\, P(x, y)\mathcal{O}(x + iy)$$

Introduction to complex Langevin (2/2)

A *less* naive generalization of real Langevin

- **Expectation values with complex Langevin:**

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

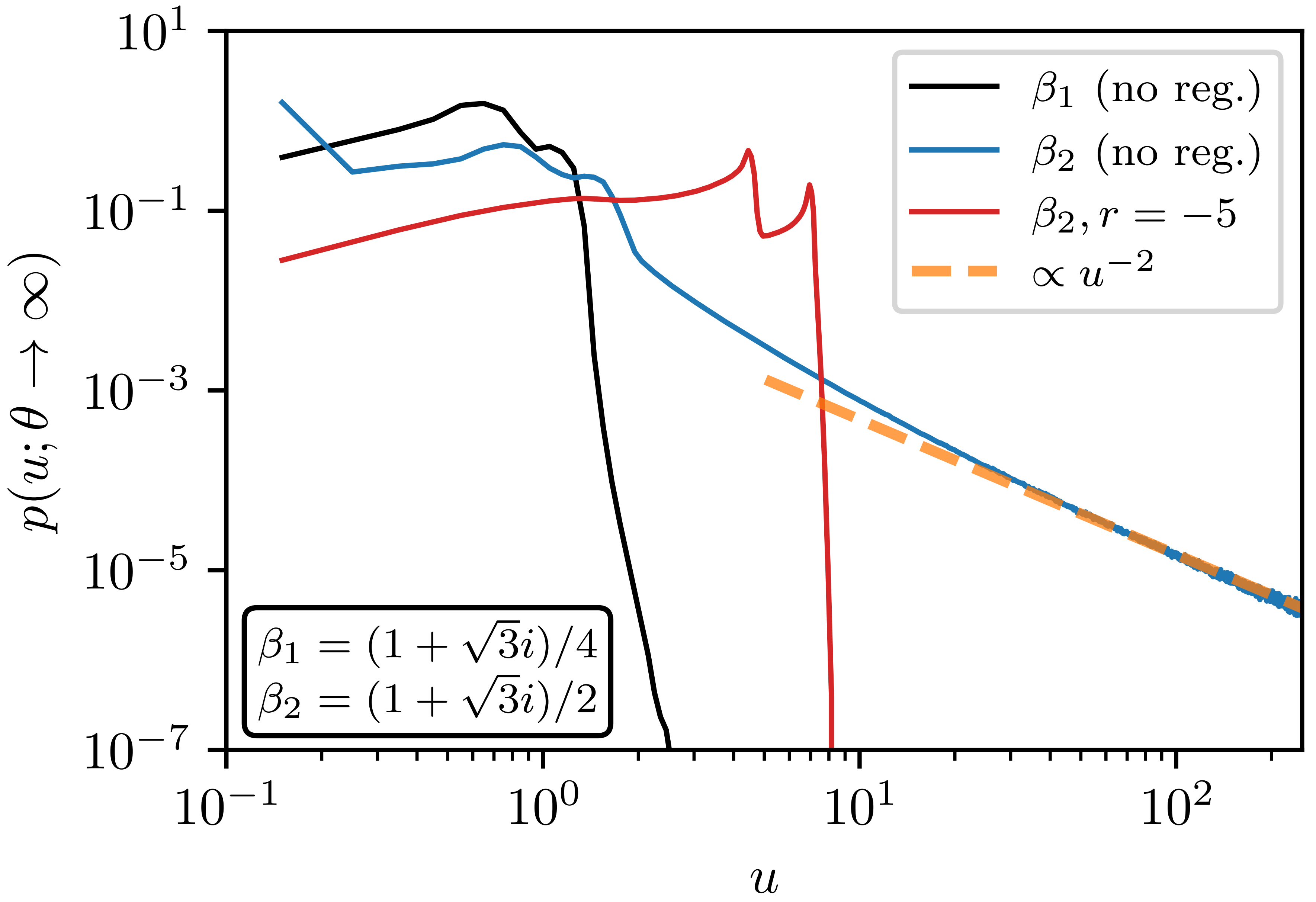
- Correspondence to Fokker-Planck equation: $\partial_\theta P(x, y; \theta) = L^T P, \quad L^T = \partial_x(\partial_x + \mathrm{Re}K) + \partial_y \mathrm{Im}K$

We solve that directly for simple models!

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

[K. Nagata et al: *Phys.Rev.D* 94 (2016) 11, 114515]

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



- **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):

$$D_\sigma := \{z(t_f) \in \mathbb{C} :\ z(-\infty) = z_\sigma, \dot{z}(t_f) = -\overline{S}'(z(t_f))\}$$

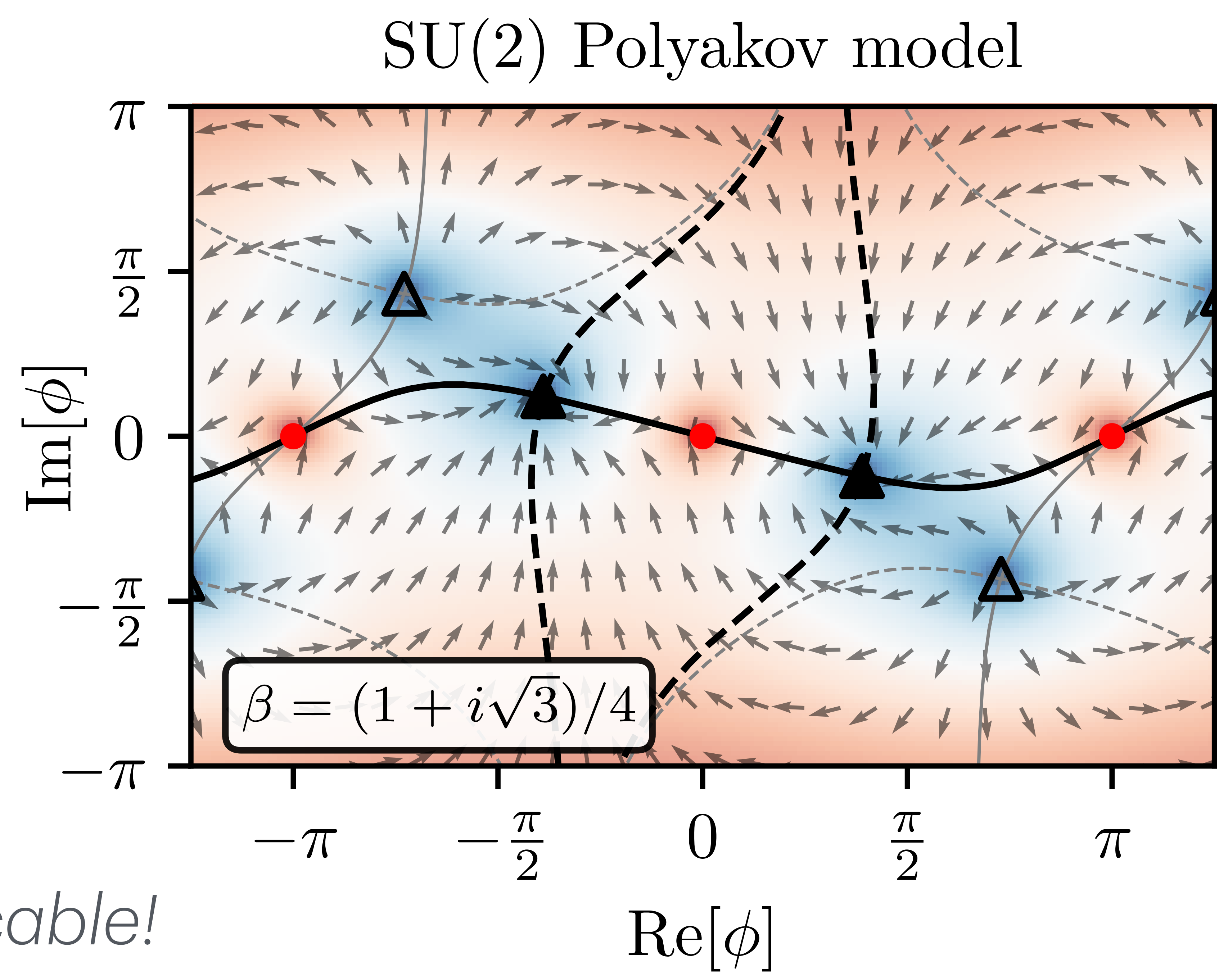
- Co-thimbles (SA paths):

$$K_\sigma := \{z(t_f) \in \mathbb{C} :\ z(-\infty) = z_\sigma, \dot{z}(t_f) = \overline{S}'(z(t_f))\}$$

- **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 is applicable!

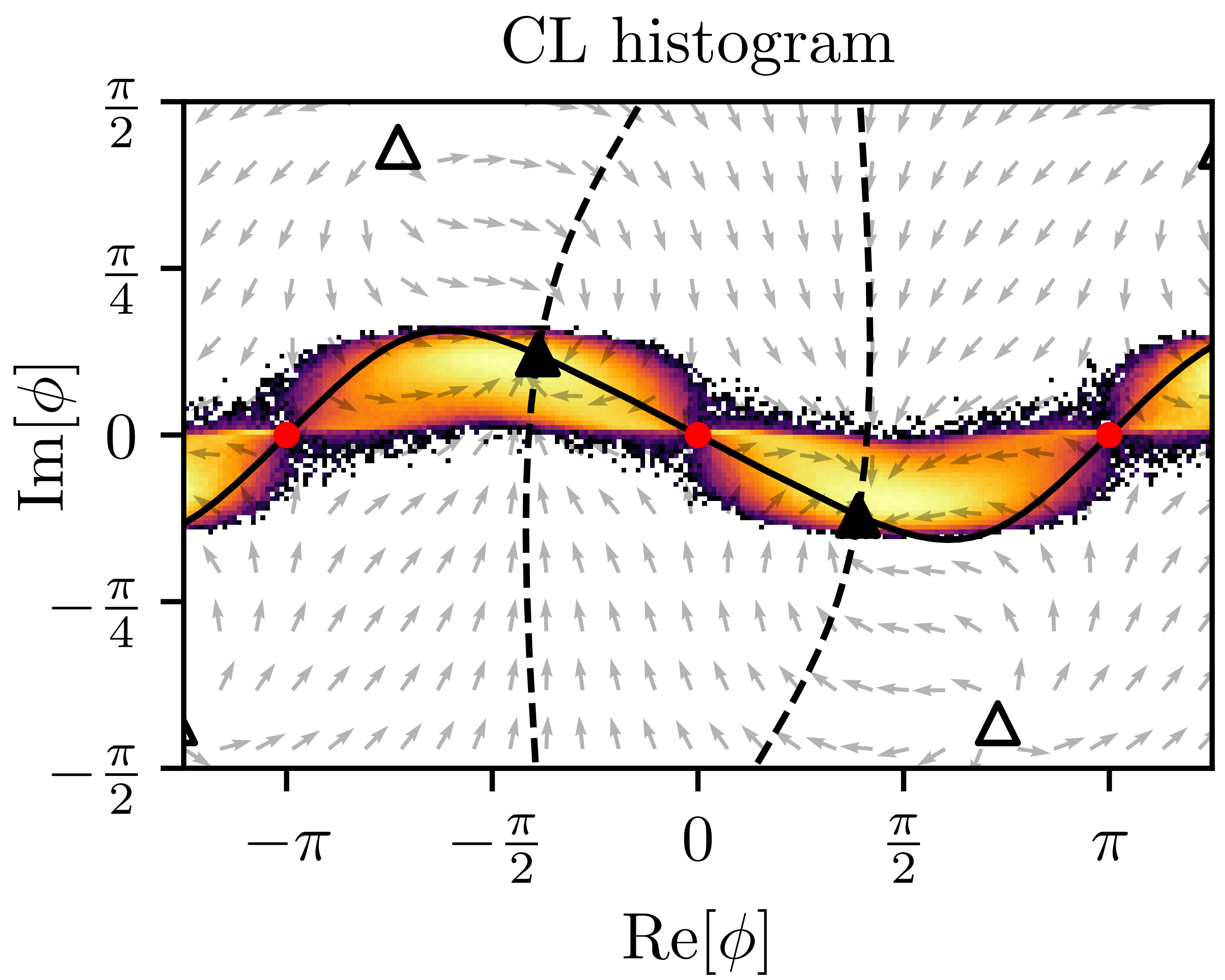


Nothing but intuition and a hunch...

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 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 find regularizations for complex Langevin!***

The 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

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

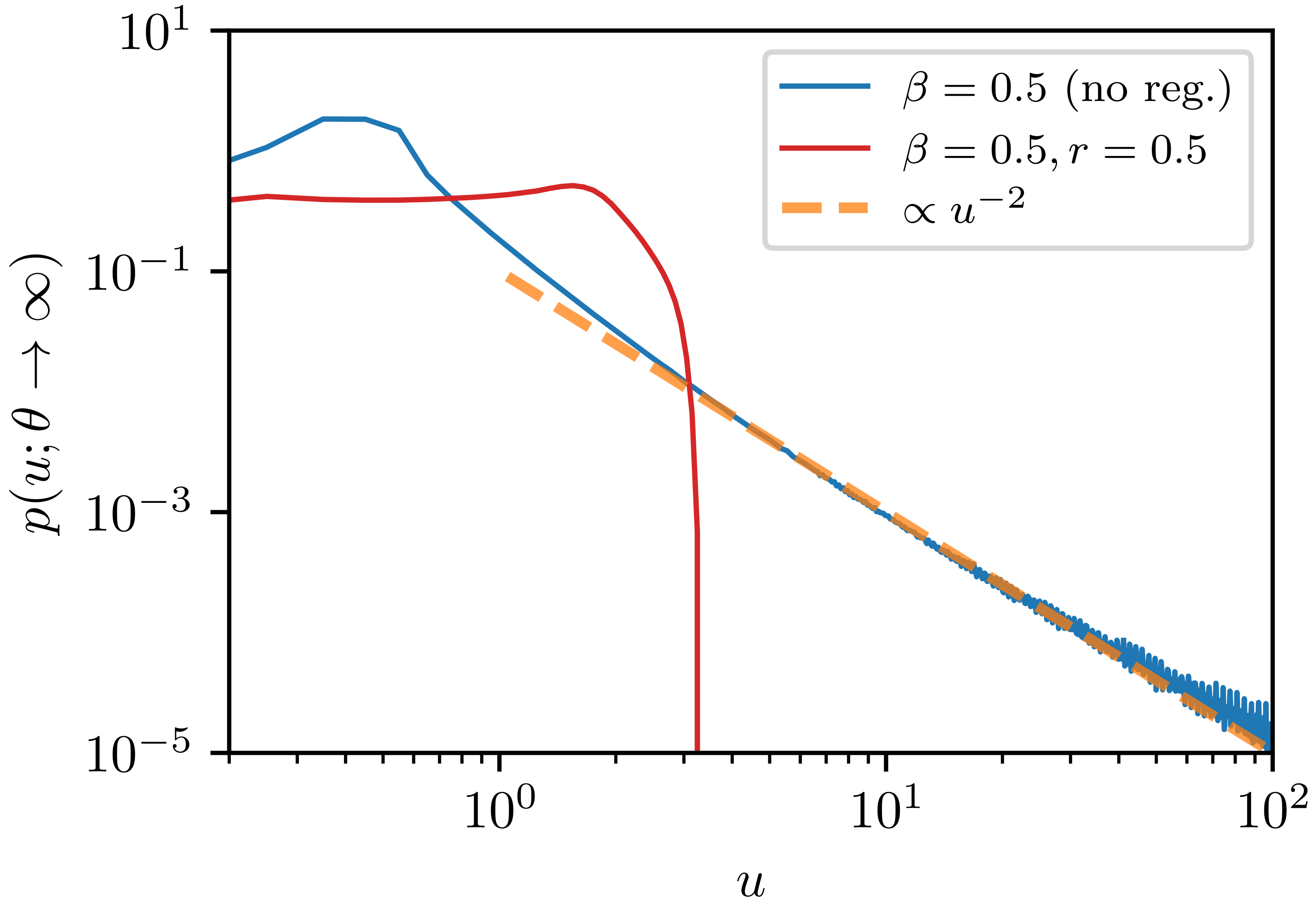
- **Criterion of correctness is not satisfied:**
  - Emergence of boundary terms [D. Sexty et al arXiv:1808.05187]
  - Decay of density of drift magnitude (right figure) [K. Nagata et al: *Phys.Rev.D* 94 (2016) 11, 114515]

- Analytic expectation values (bottom figure):

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

Observables: $\mathcal{O}_k(x) = \cos(x)^k$

Order k	$\mathrm{Re}\langle\mathcal{O}_k\rangle_\rho^{\mathrm{exact}}$	$\mathrm{Re}\langle\mathcal{O}_k\rangle_\rho$	$\mathrm{Im}\langle\mathcal{O}_k\rangle_\rho^{\mathrm{exact}}$	$\mathrm{Im}\langle\mathcal{O}_k\rangle_\rho$
1	0	-0.38(2)	-0.258153	-12.22(6)
2	0.483695	$-1.541(7)\times10^{4}$	0	$1.15(9)\times10^{3}$
3	0	$2.2(1)\times10^{6}$	-0.192932	$1.45(2)\times10^{7}$
4	0.358716	$5.3(2)\times10^{9}$	0	$-3.1(3)\times10^{9}$
5	0	$-2.6(3)\times10^{12}$	-0.160492	$1.39(5)\times10^{13}$
6	0.297246	$3.51(5)\times10^{16}$	0	$-1.3(8)\times10^{15}$



Thimbles of the cosine model

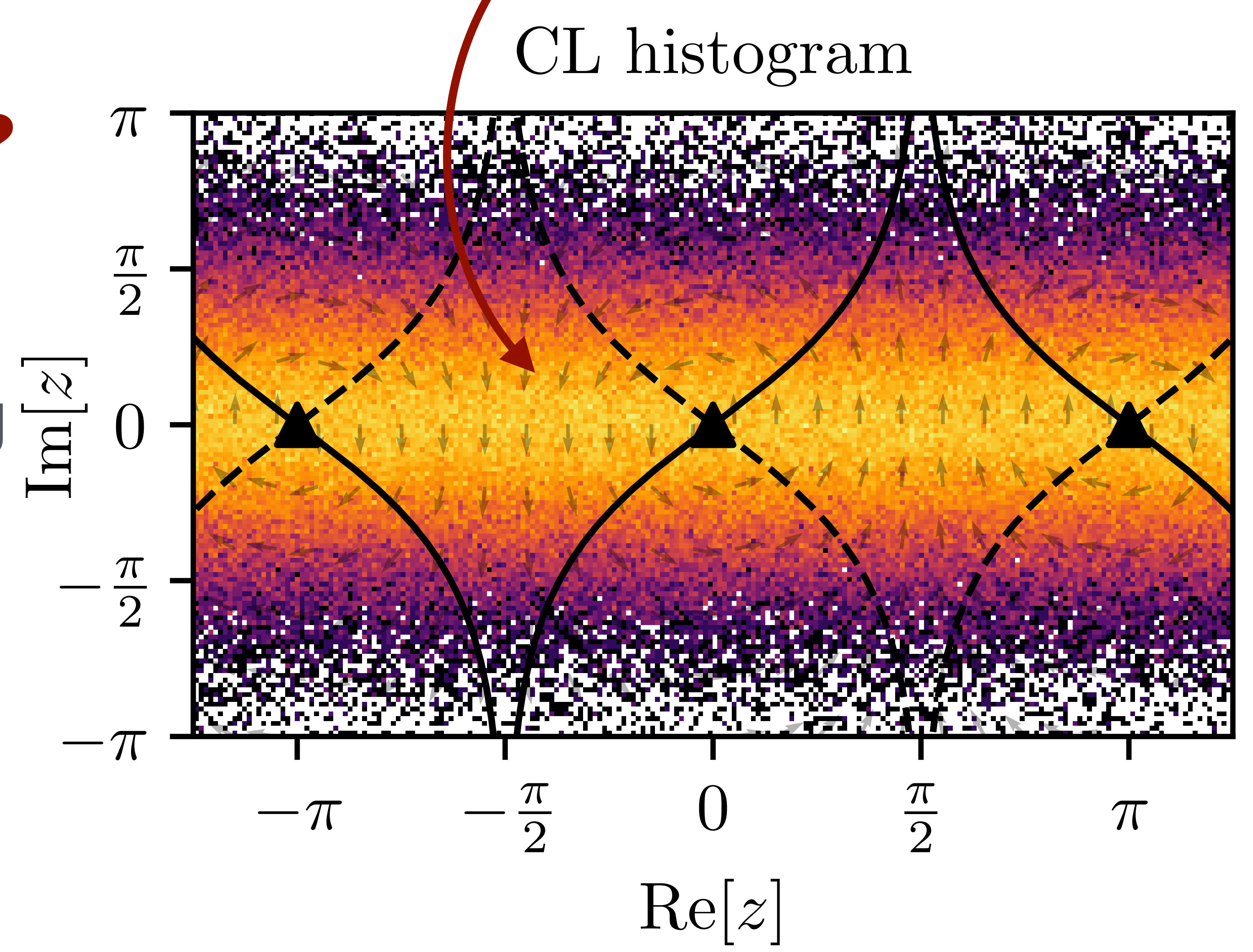
Simple structure with obvious consequences

- 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
- **What features of a theory lead to failure/success of CL?**

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



Designing weight regularizations

If you cannot simulate the theory — change the theory

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

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

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

…

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

1. **Only one relevant stationary point** should be **"close" to the real line**

2. **Singularities** that connect to contributing thimbles should be **at the real boundary of D**

3. We want to **avoid any asymptotic structure** of contributing thimbles ("tamed" thimbles)

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**

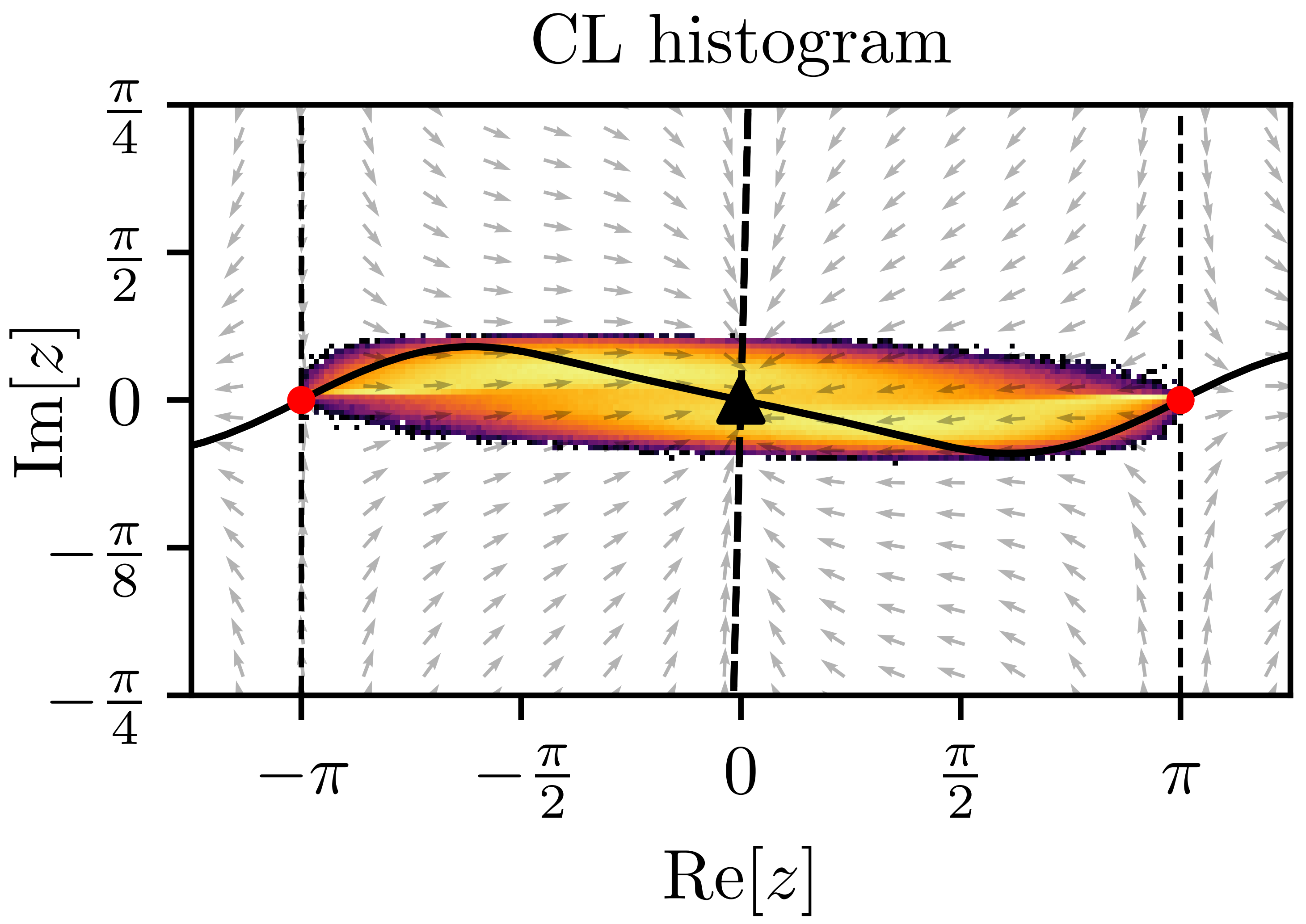
$$\rho_R(x) = e^{i\beta\cos(x)} + R(x)$$

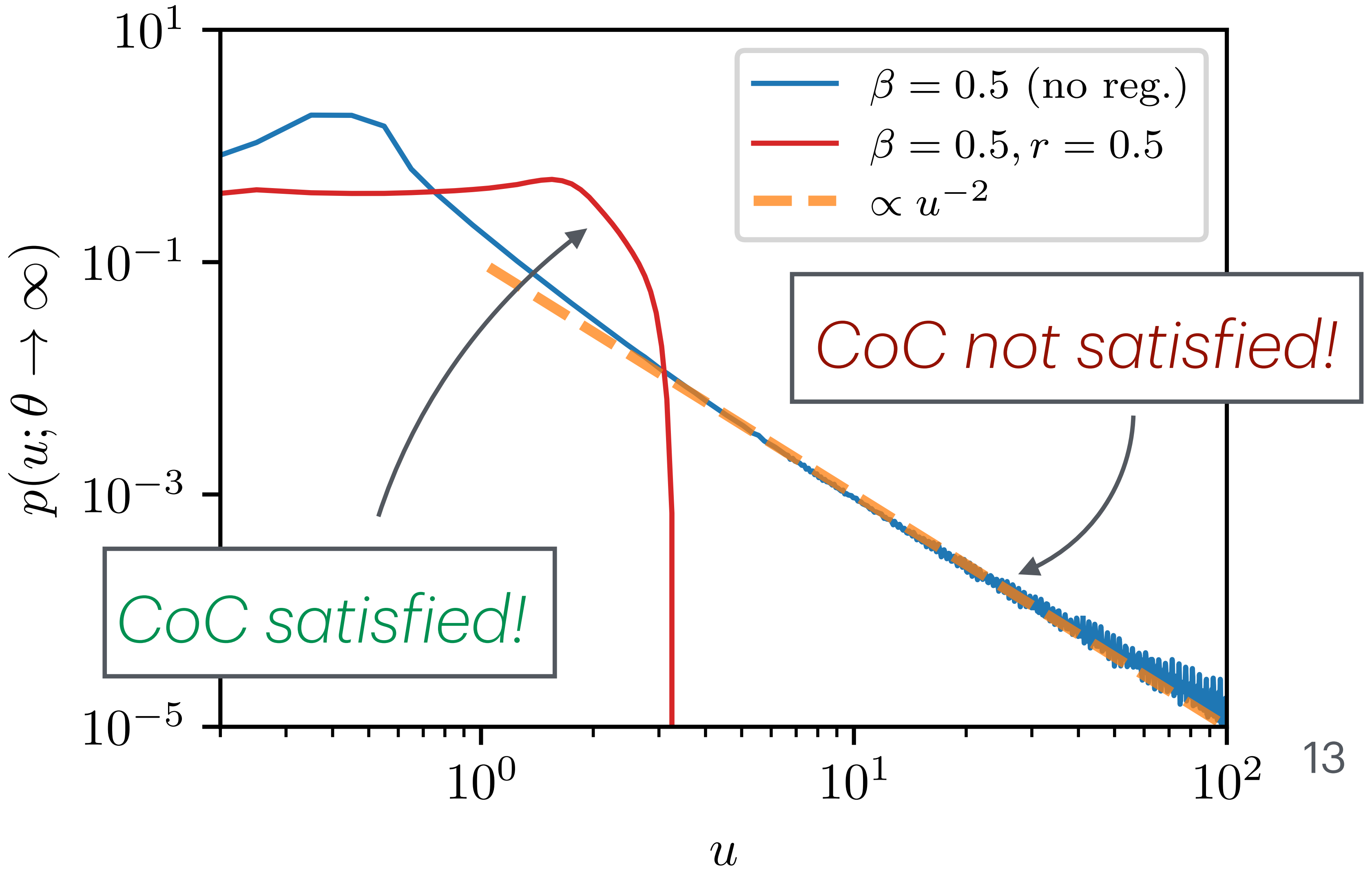
$$R(x) = r(x^2 - \pi^2) - \exp(i\beta), r \in \mathbb{C}$$

  - Break periodicity and periodic continuation breaks holomorphicity
  - Boundary at $\mathrm{Re}(z) = \pm\pi$ is repulsive and does not contribute!

- **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:

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





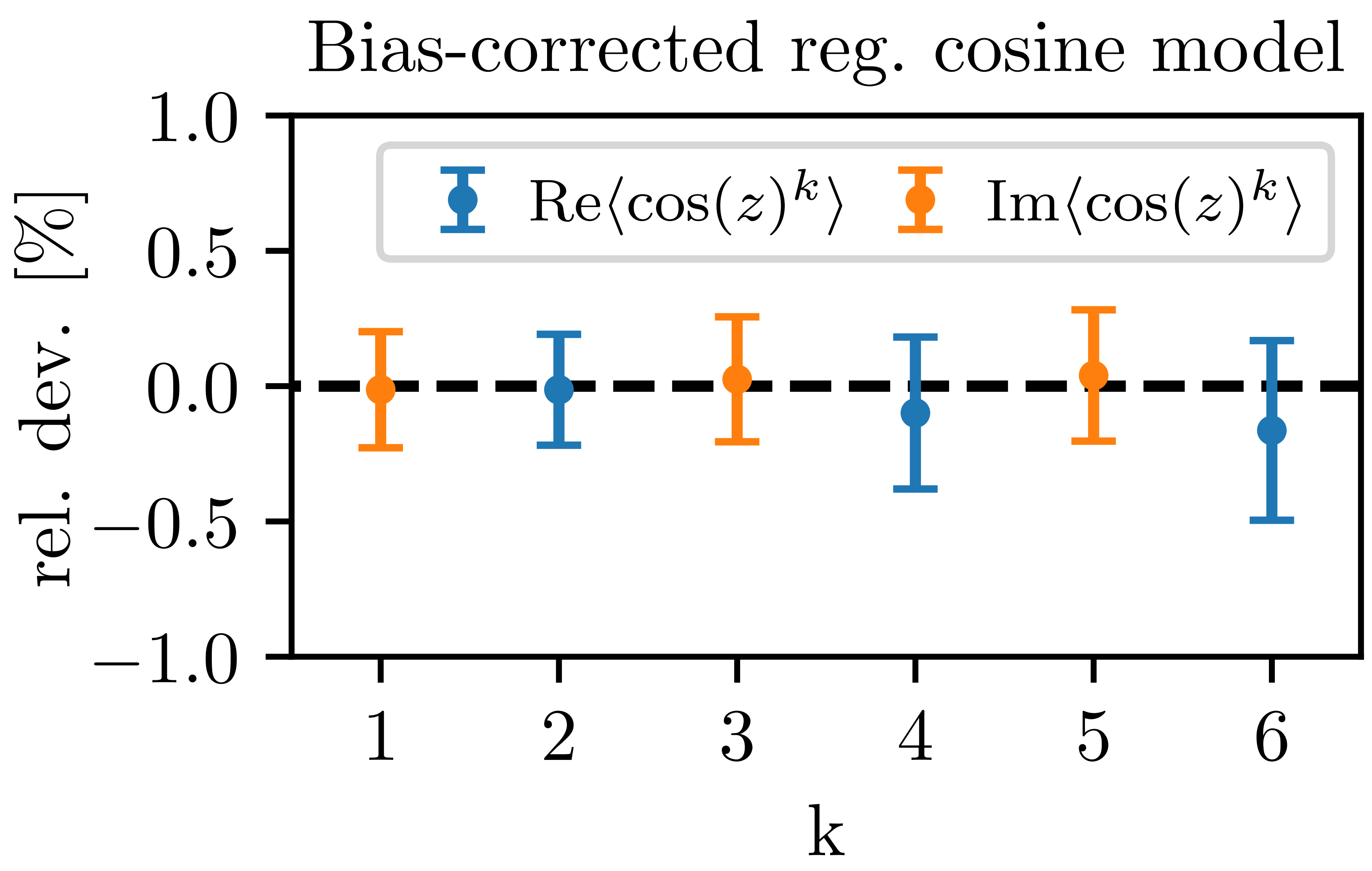
Corrections for regularizations

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

Potential problem: vanishing for $r \to \infty$!

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

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

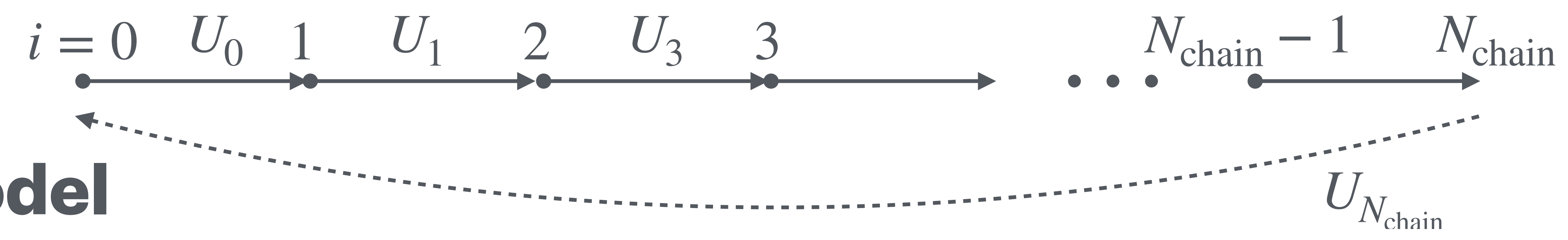
Reduced Polyakov loop model (1/2)

Reducing a 'gauge theory' to a 'scalar theory'

- **Polyakov loop action** in SU(2):

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

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



- Gauge freedom leads to equivalence to the **one-link model**

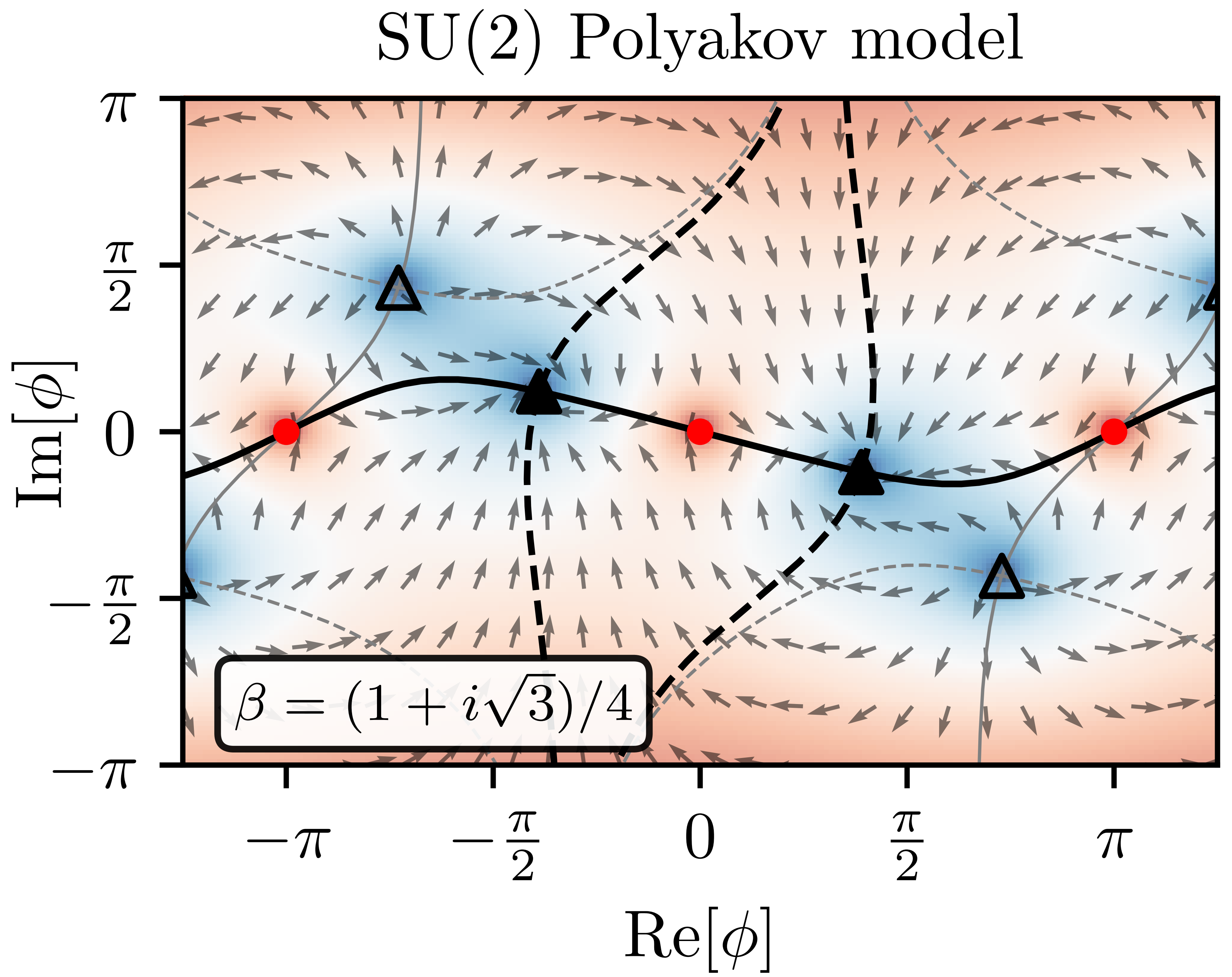
- **Haar measure** can be reduced

$$\int_{SU(2)} dU\, e^{\beta \mathrm{Tr}(U)} \rightsquigarrow \int_{-\pi}^{\pi} dx\, \sin^2(x)\, e^{2\beta\cos(x)}$$

- Translating **observables** and **effective action**

$$S(x) = -2\beta\cos(x) - \ln(\sin(x)^2), \qquad \mathrm{Tr}(U) \leftrightarrow 2\cos(x)$$

- **Compact domain** of integration $D = [-\pi, \pi]$

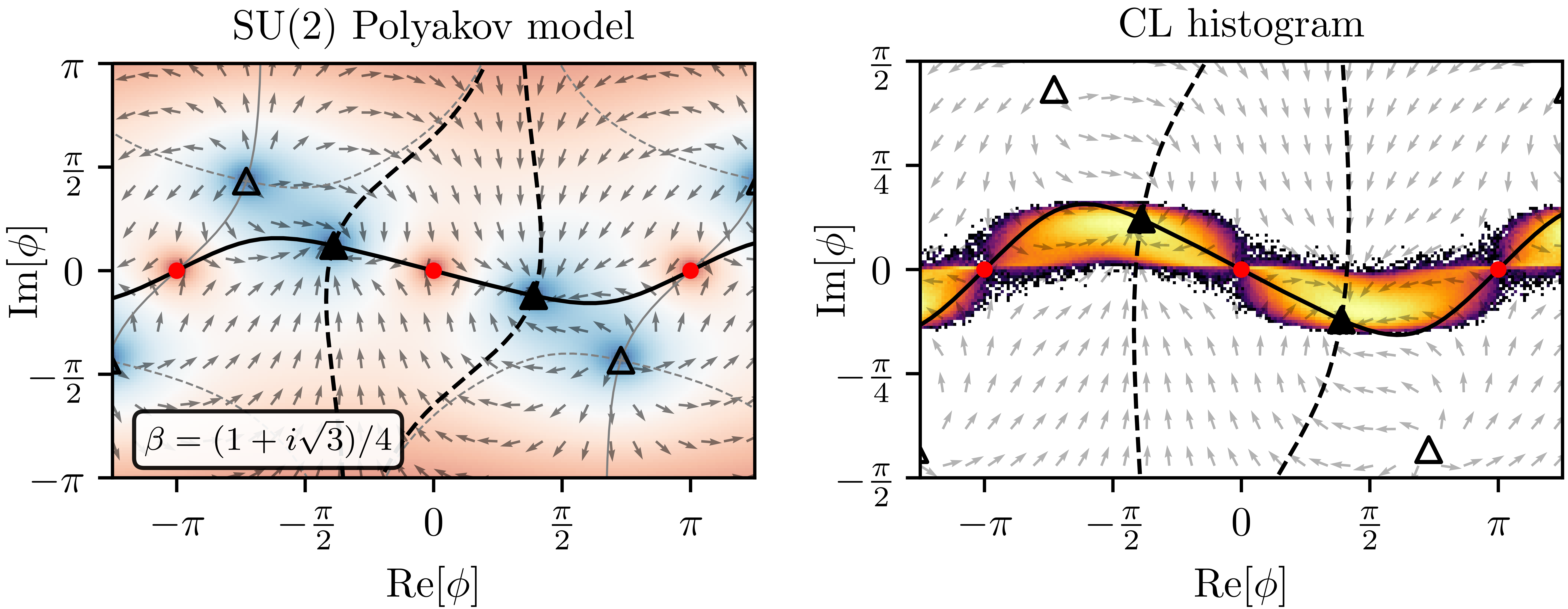


Reduced Polyakov loop model (2/3)

For small-magnitude couplings, CL works…

- For $\beta = \left(1 + i\sqrt{3}\right)/4$ (up to point symmetry) only one thimble contributes

  → sharp histogram/density → CL converges correctly

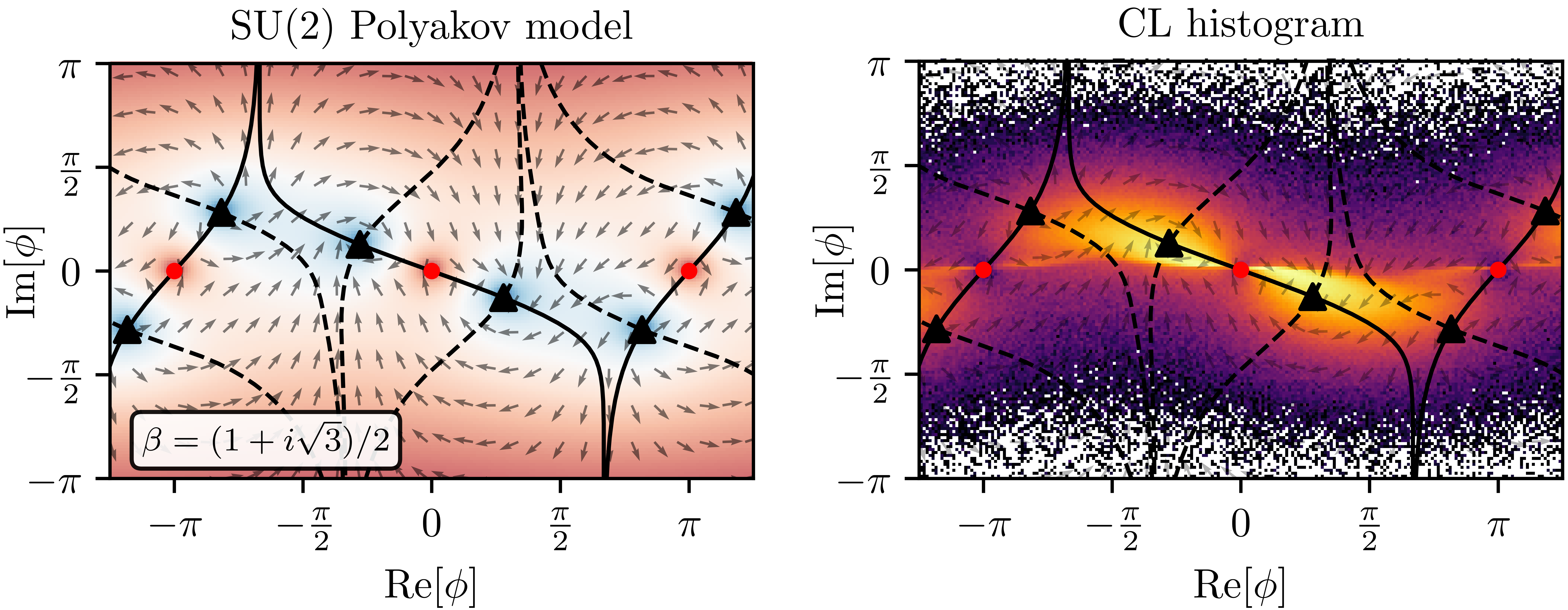


Reduced Polyakov loop model (3/3)

... for large-magnitude couplings, it doesn't.

- For $\beta = \left(1 + i\sqrt{3}\right)/2$ multiple (non-compact) thimble contribute

  → slowly decaying histogram/density → CL converges wrongly



Designing weight regularizations (1/2)

Changing the Lefschetz thimble structure to achieve correct convergence

Conjecture:

The criterion of correctness of CL is satisfied if there is exactly one compact relevant Lefschetz thimble.

- **Initial situation:** The model with ρ which we want to compute exhibits multiple relevant thimbles leading to the slow decay of the drift magnitude, breaking the criterion of correctness.

- **Goal:** Find a positive definite function R, such that $\rho + rR$ has only one relevant thimble leading to a compact histogram and sufficiently fast decay of the drift magnitude.

Designing weight regularizations (2/2)

Foundation of constructing regularizations (+ some trial and error maybe)

- **Design approach:**
  1. The drift of the regularization R' should point to the real line → at large enough $|r| \to \infty$ we find R' dominating the dynamics and squeezing it to the real line
  2. Regularized weight function $\rho + rR$ zeros at the boundary which should be the only real zeros of the function
  3. Relevant thimbles have to connect to the real zeros leading to a compact thimble structure

- **Scenarios which can happen:**
  - The desired thimble structure is only achieved asymptotically at $|r| \to \infty$ — no information of original model left
  - Multiple relevant and compact thimbles are present for all r, breaking the criterion of correctness

Regularizing the reduced PLM (1/3)

Two potentially viable candidates for regularizations

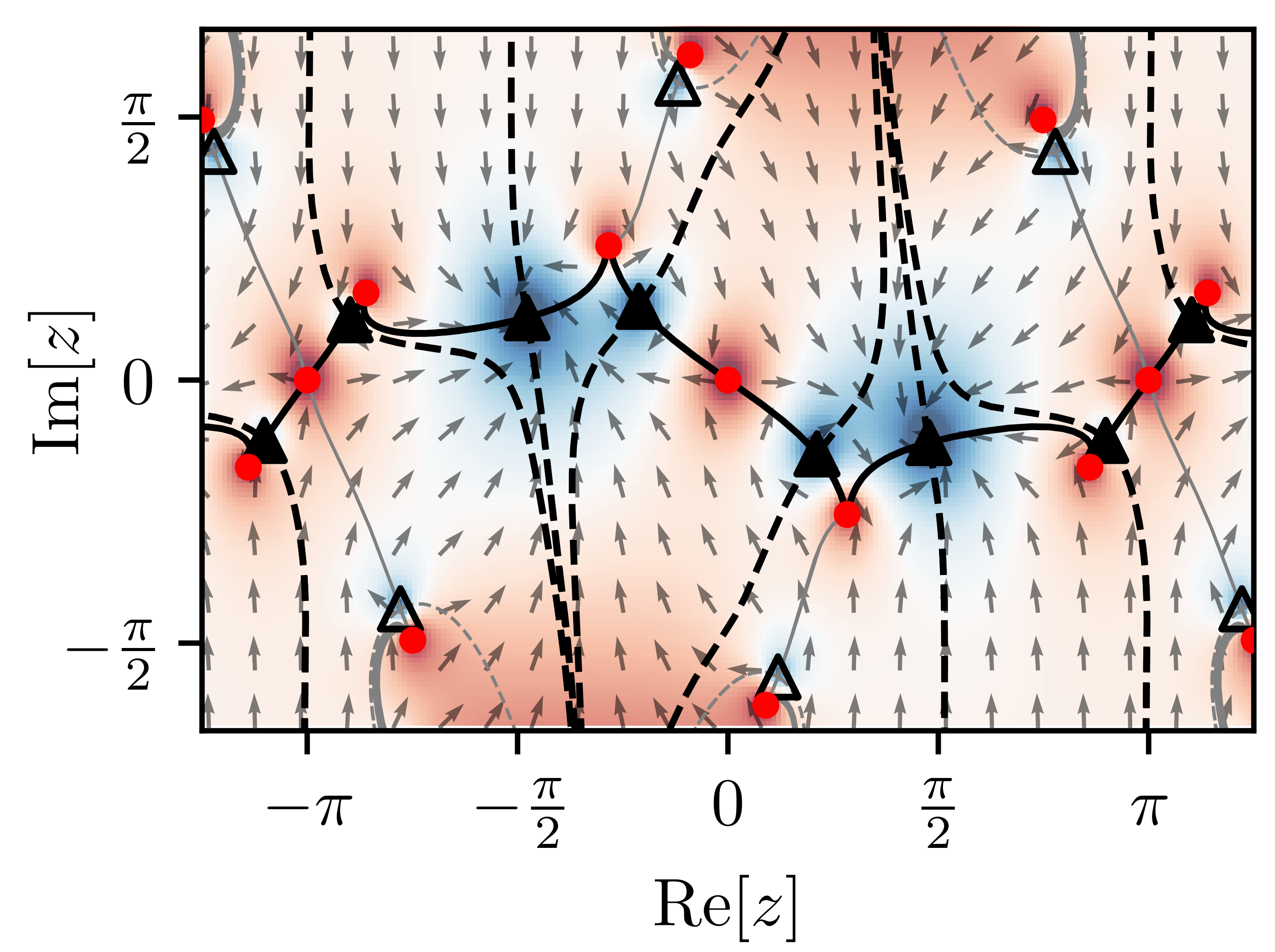
- Weight function of reduced PLM: $\rho = \sin^2(x) e^{2\beta \cos(x)}$

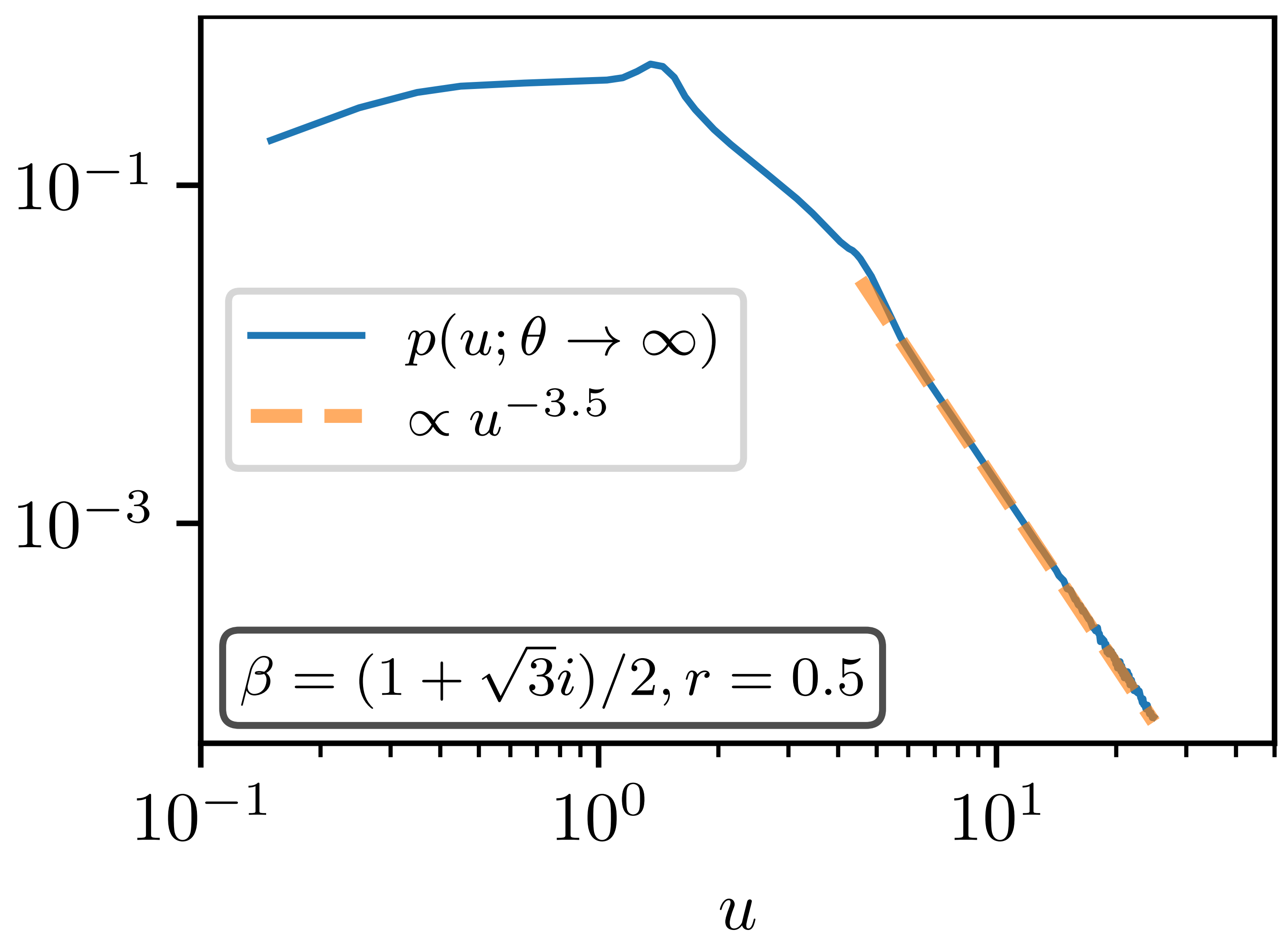
  Haar measure $dU \hat{=} \sin^2(x) dx$

- Two candidates that follow the design approach:

1. Same as for the cosine model: $R_1(x) = x^2 - \pi^2$ (right)
   - Desired drift properties, pointing towards the real line
   - Eliminates zero at the origin from he Haar measure
   - BUT: multiple thimble structure for all r (top figure), ➞ criterion is broken (bottom figure) despite compact structure

2. Periodic regularization: $R_2(x) = \cos(x) + 1$ (next slide)



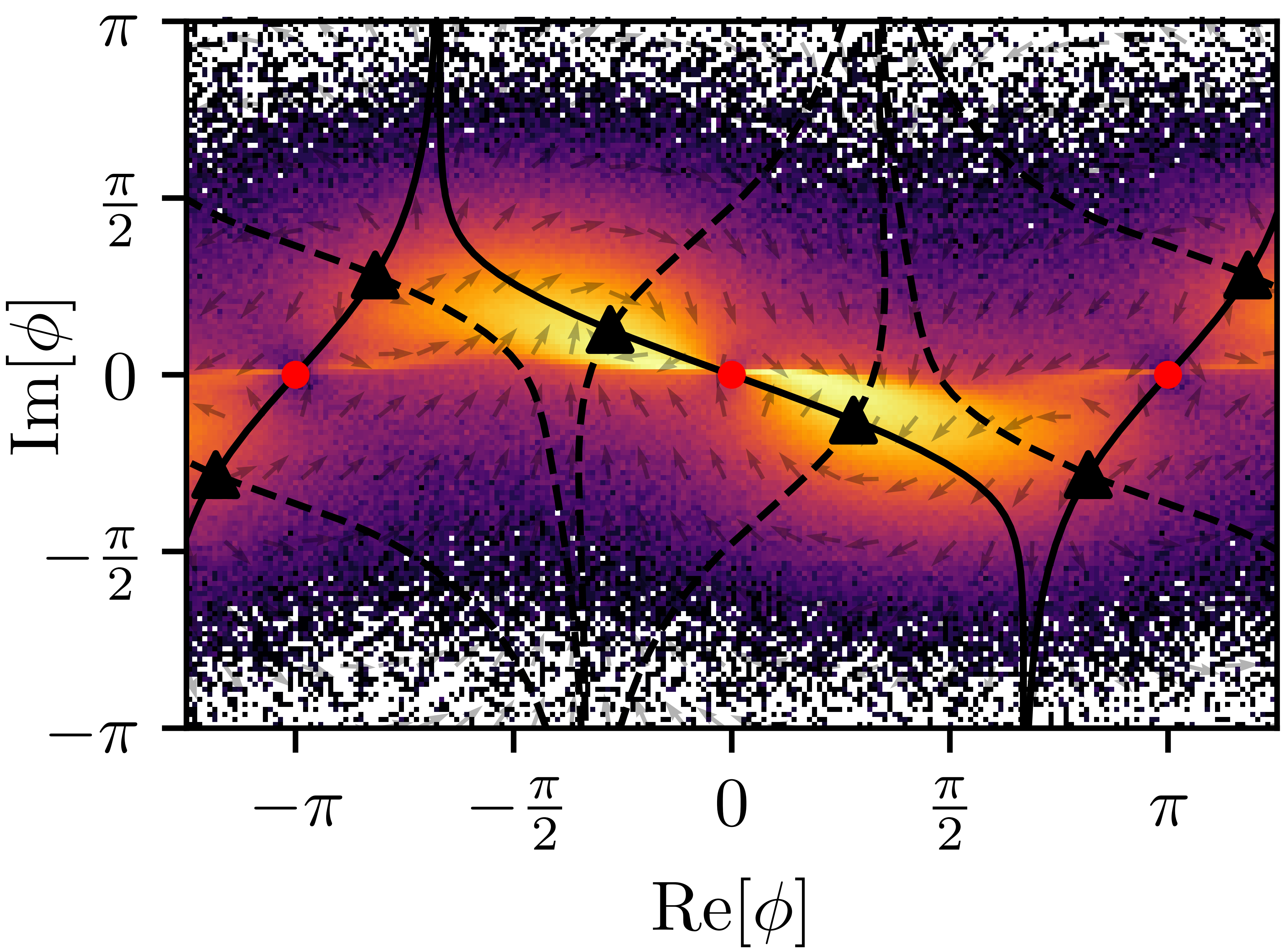


Regularizing the reduced PLM (2/3)

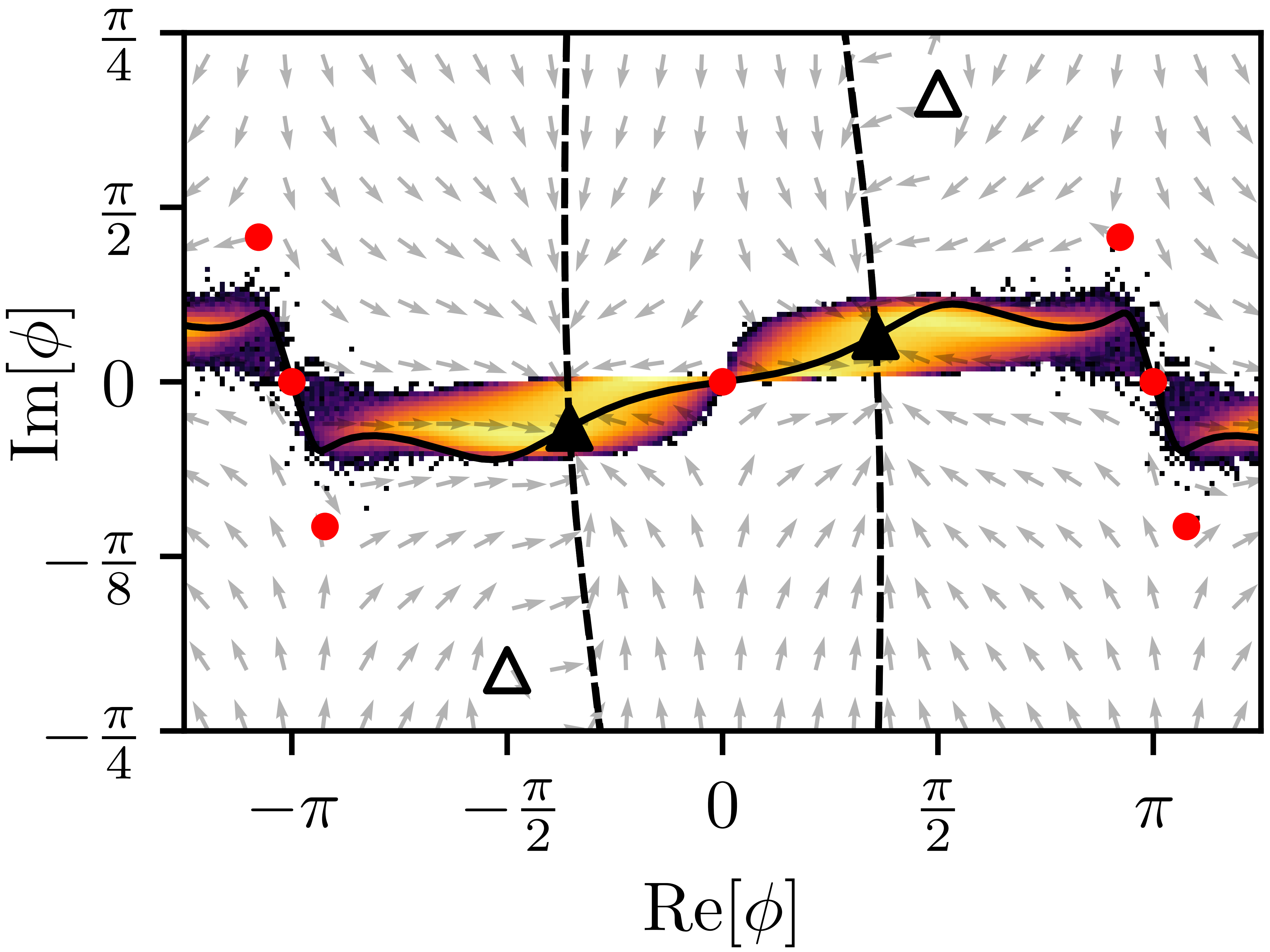
Squeezing/'Compactification' of CL histogram via regularization term

- Regularization $R(x) = \cos(x) + 1$ achieves desired thimble structure → correct convergence

No regularization



<u>With</u> regularization

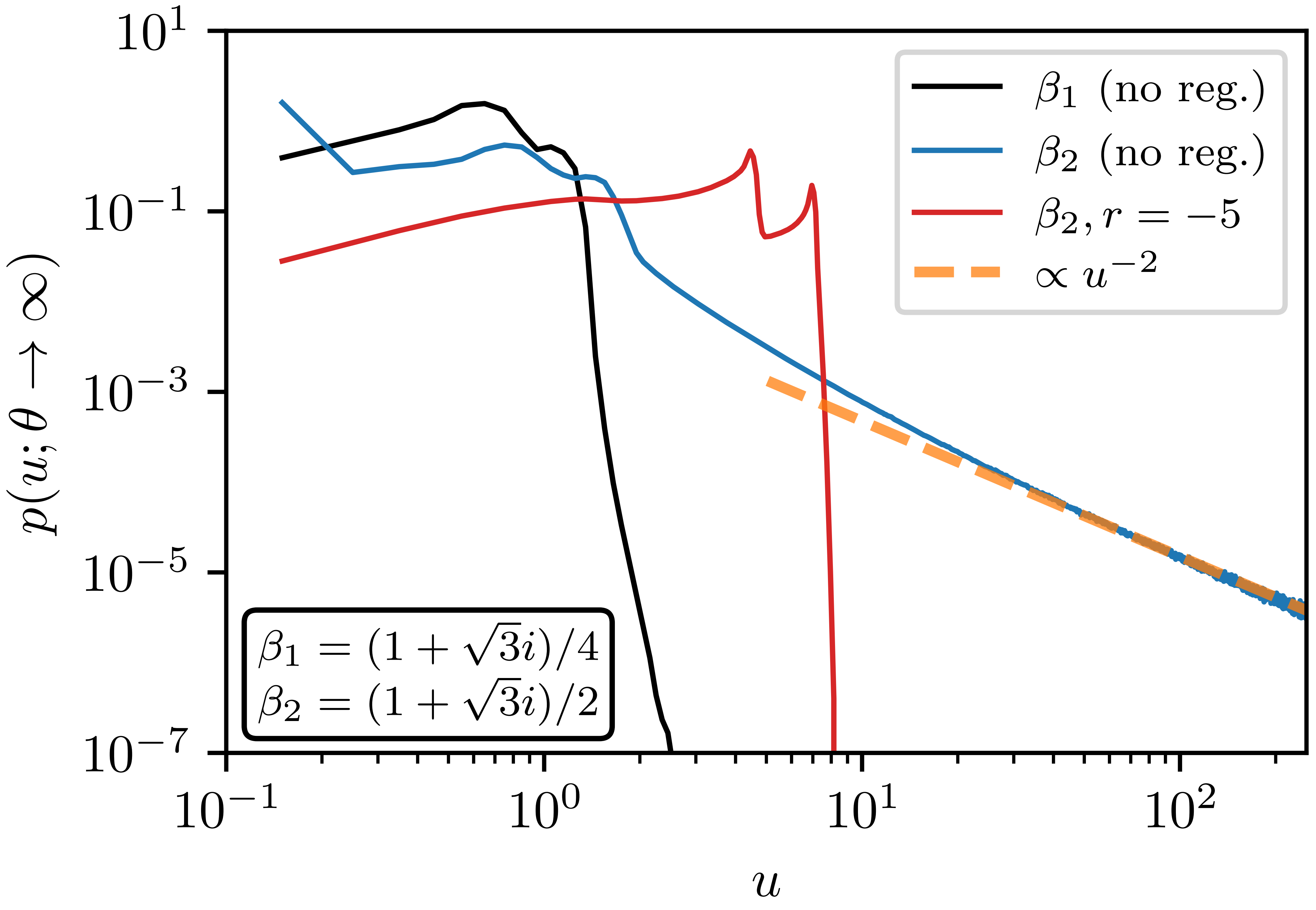


Regularizing the reduced PLM (3/3)

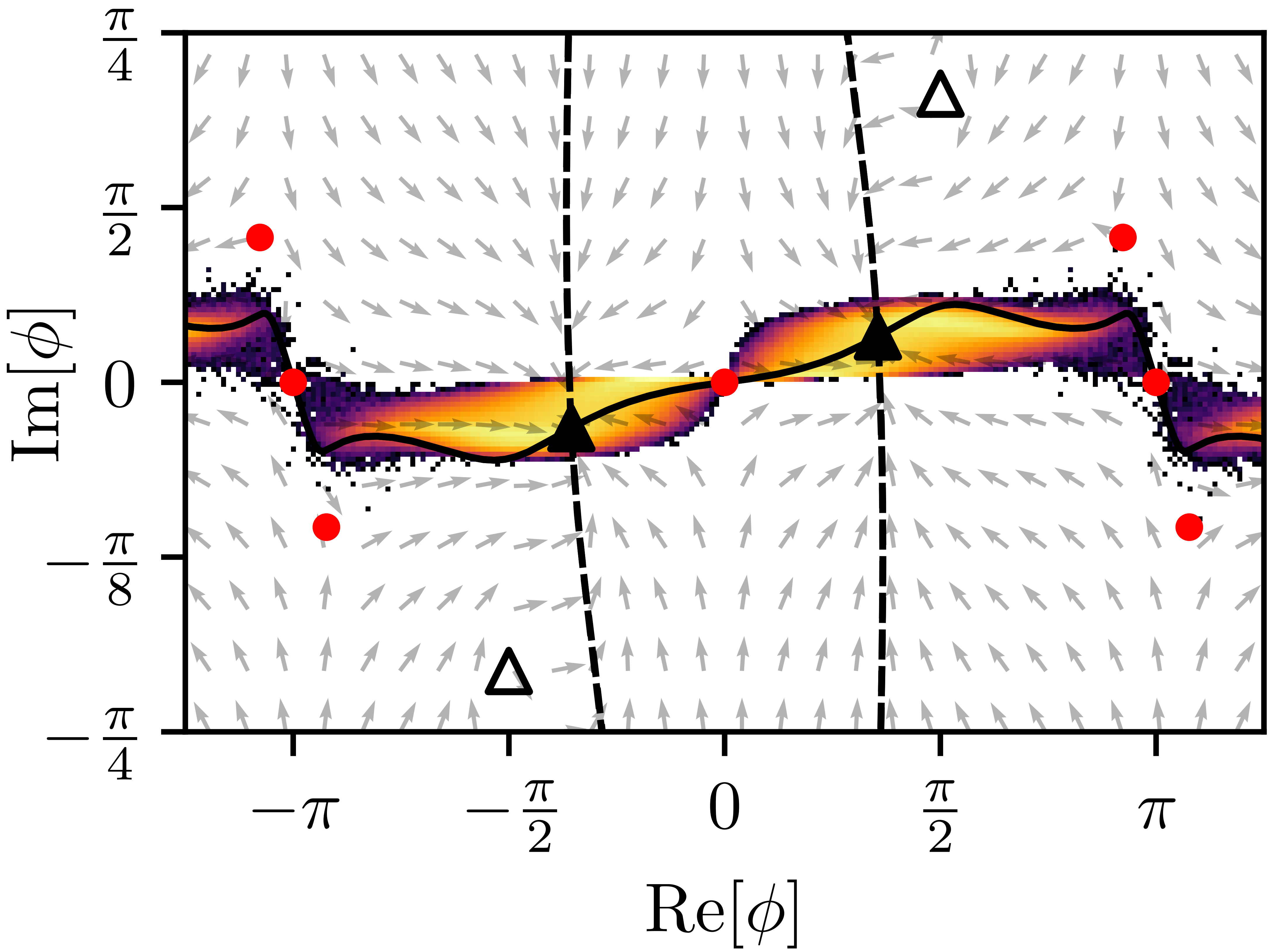
Regularization term cures the criterion of correctness

- Regularization $R(x) = \cos(x) + 1$, $r = -5$ leads to exponential decay of drift magnitude density

Drift magnitude density



With regularization



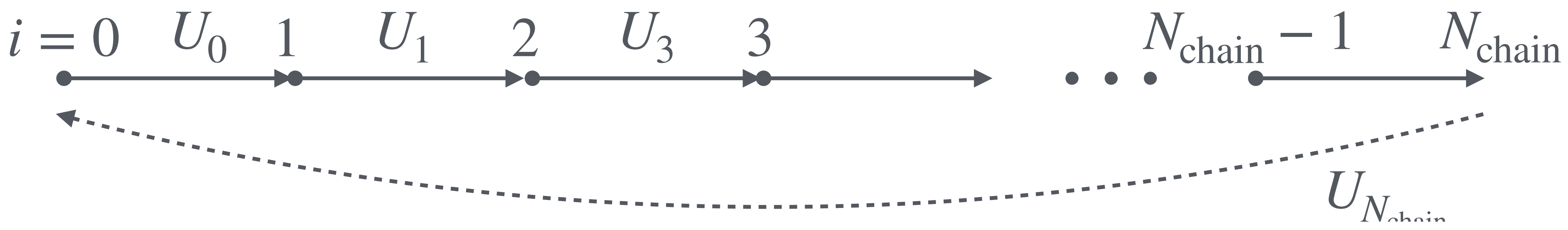
Regularizations in SU(2) (1/2)

Translating back from the reduced model to the SU(2) link-formulation

- **Polyakov loop action** in SU(2):

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

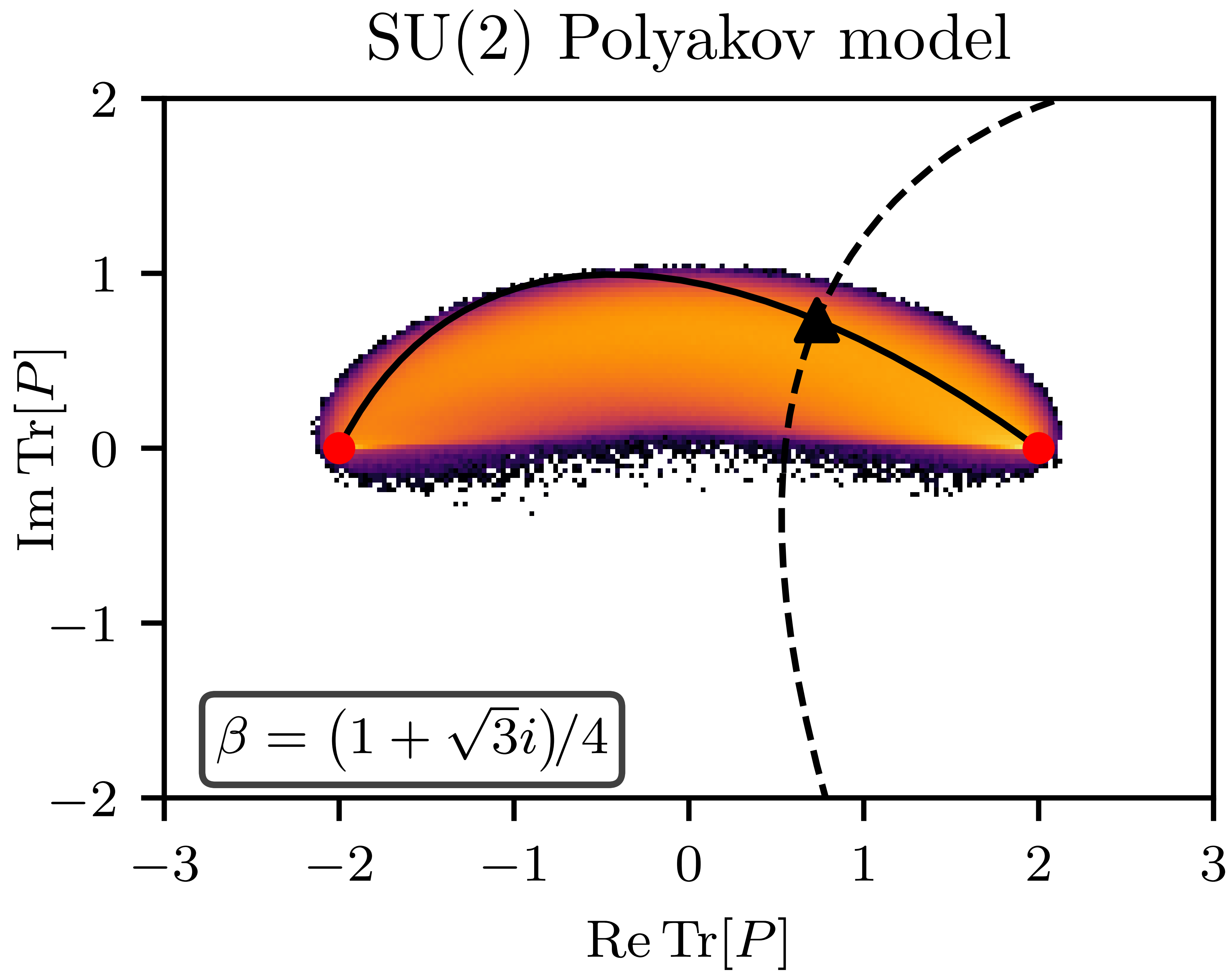
$$P = \prod_{i=0}^{N_\mathrm{chain}} U_i, \quad U_i \in \mathrm{SU}(N_c)$$



- Regularization $R[P] = \mathrm{Tr}[P]/2 + 1, \quad \mathrm{Tr}[P] \in [-2,2]$

- We simulate a chain with $N_\mathrm{chain} = 64$ links

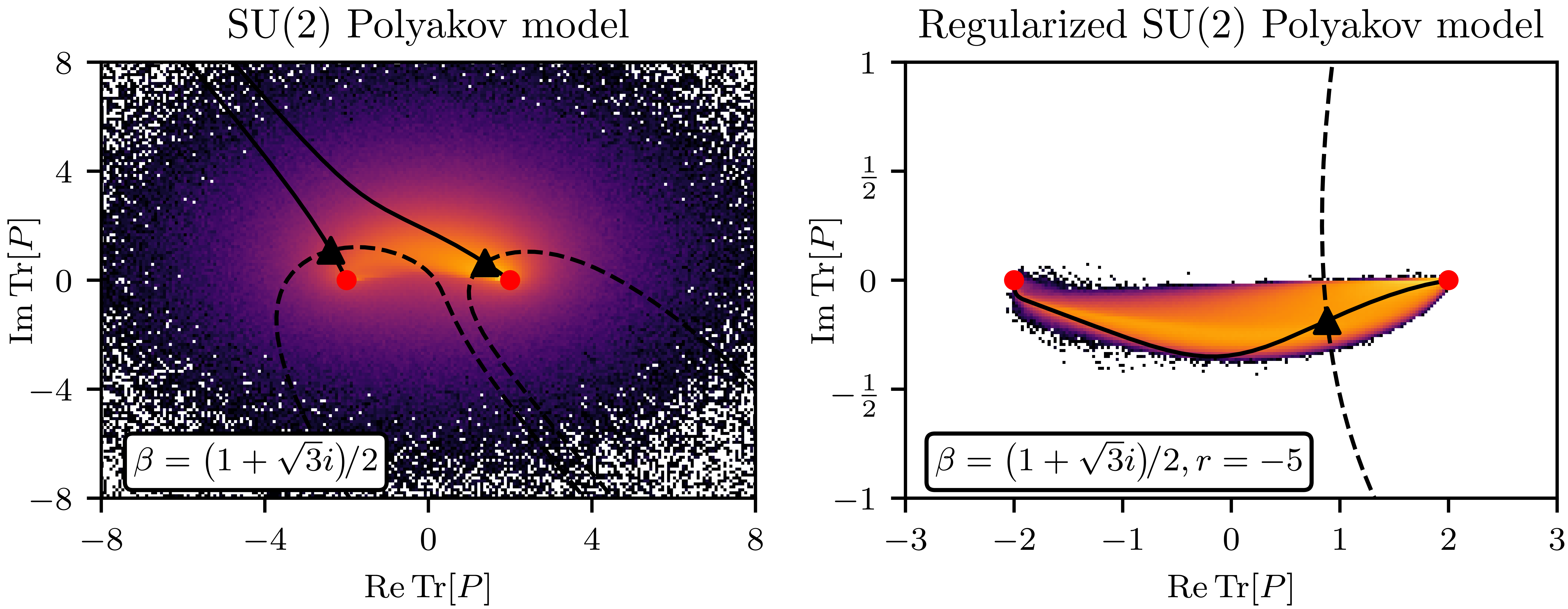
- Note: complexification yields $SU(2) \rightsquigarrow SL(2,\mathbb{C})$
  - ✳ iterative gauge transformation ('gauge cooling')
  - ✳ minimize unitarity norm $F[U] = \sum_i \mathrm{Tr}[UU^\dagger - 1]$



Regularizations in SU(2) (2/2)

Our approach in conjunction with gauge cooling works also for SU(2)

- Regularization $R[U] = \mathrm{Tr}[U]/2 + 1$ achieves desired thimble structure
  → sharp histogram/density → correct convergence



Generalization to the SU(3) Polyakov loop model:
Applying the same ideas to a different group

The Polykov chain in SU(3) (1/2)

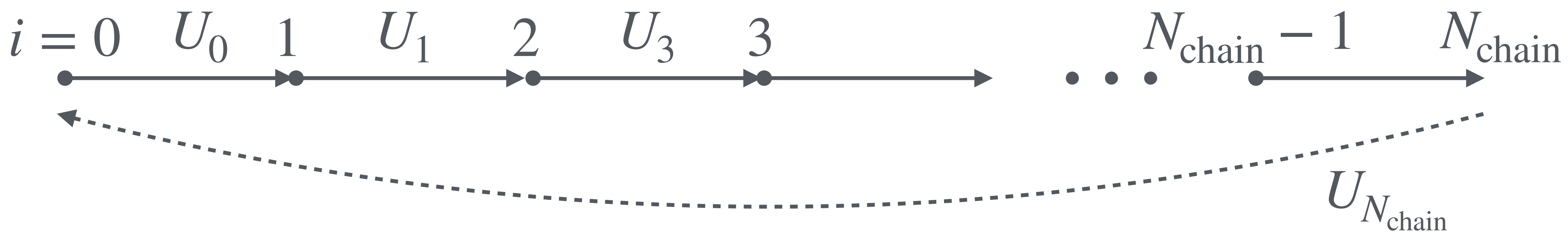
Similarities with finite density QCD

- Action for the SU(3) PLM

$$S = -\left(\beta + \kappa e^{-\mu}\right) \mathrm{Tr}[P] - \left(\beta + \kappa e^{\mu}\right) \mathrm{Tr}[P^{-1}]$$

  - Couplings $\beta, \kappa \in \mathbb{R}$
  - Chemical potential $\mu \in \mathbb{R}$

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



- Source of sign problem:

  Traces of the Polyakov loops are complex; for $\kappa \neq 0$ and $\mu \neq 0$ we have $\mathrm{Tr}[P] \neq \mathrm{Tr}[P^{-1}]$

- **Sign-problem is rather weak → solvable using CL with gauge cooling**

- **To make it harder we consider imaginary couplings $\beta \in i\mathbb{R}$**

  → *may be interpreted as real-time scenario with finite chemical potential*

The Polykov chain in SU(3) (2/2)

Reduction of the Haar measure leads to a more complicated situation for the thimbles

- We can reduce the Haar measure of SU(3)

$$dU \mathrel{\hat{=}} d\phi_1 d\phi_2 \sin^2\left(\frac{\phi_1 - \phi_2}{2}\right)\sin^2\left(\frac{\phi_1}{2} + \phi_2\right)\sin^2\left(\phi_1 + \frac{\phi_2}{2}\right), \quad \phi_1, \phi_2 \in [-\pi, \pi]$$

$$P \mathrel{\hat{=}} \mathrm{diag}\left(e^{i\phi_1}, e^{i\phi_2}, e^{-i(\phi_1+\phi_2)}\right)$$

- To analyze the Lefschetz thimble via the reduced model we need to complexify both angles:
  ➞ four-dimensional space — simple to do but no nice figures

- We conduct simulations directly for SU(3) — but the Haar measure serves as guide for the design of the regularization (next slide)

Construction of regularizations in SU(3)

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

- The regularized weight function $\rho + R$ has the only zeros on the boundary of the domain of integration
  - Boundary of the domain of integration: $(\phi_1^*, \phi_2^*) \in \pm\pi \times [-\pi, \pi]$ or $[-\pi, \pi] \times \pm\pi$
  - Zeros of the Haar measure: $\phi_1^* = -\phi_2^*/2,\ \phi_1^* = -2\phi_2^*,\ \phi_1^* = \phi_2^*$
- At these points, the trace of the Polyakov loop takes three different values

$$\mathrm{Tr}[P^{\pm 1}] = e^{i\phi_1^*} + e^{i\phi_2^*} + e^{-i(\phi_1^*+\phi_2^*)} \in \{-1, -1+2i, -1-2i\}$$

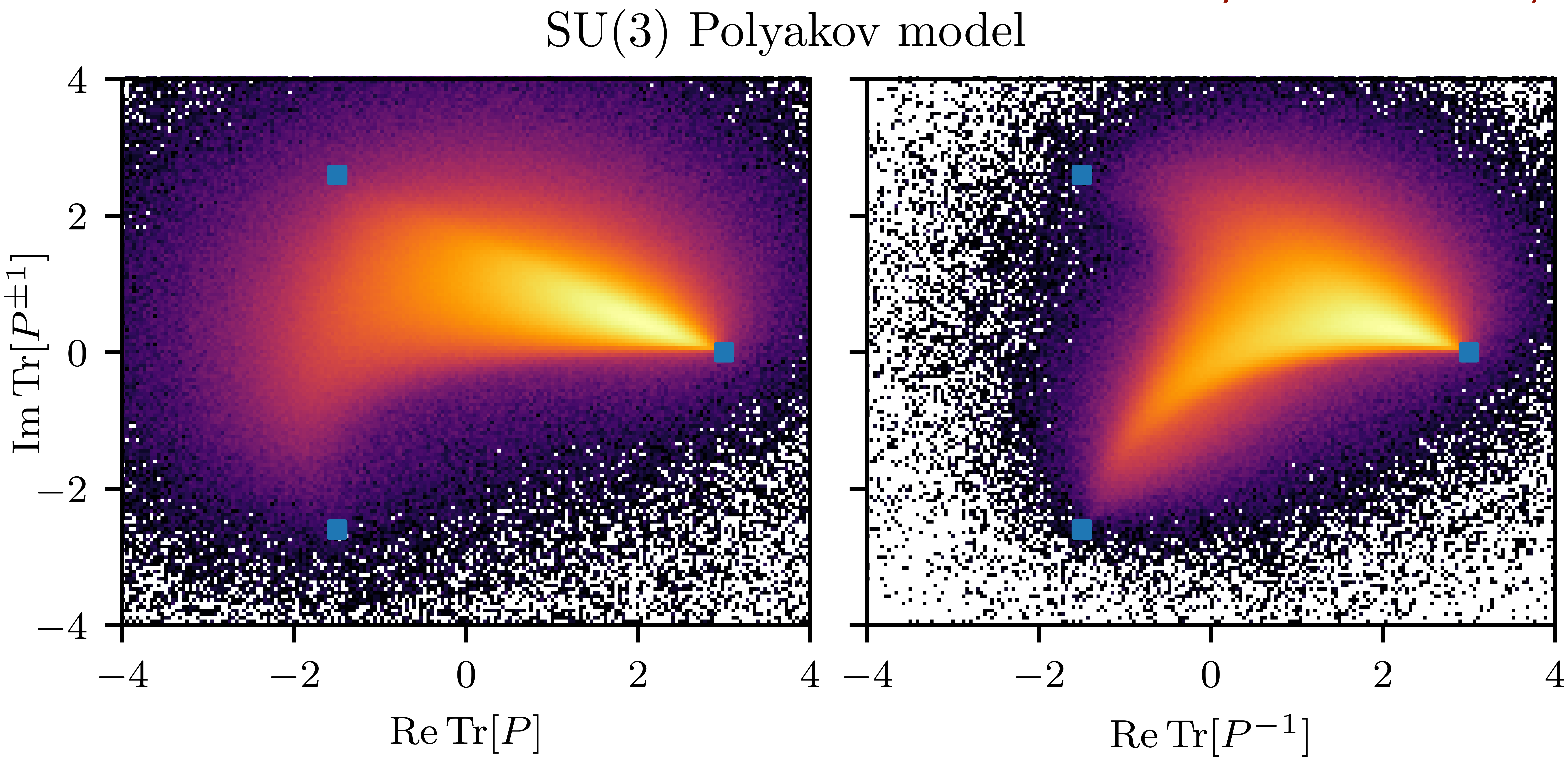
✳ **Regularization for SU(3) Polyakov chain model**

$$R[P] = r\, q(+1)\, q(-1),$$
$$q(\sigma) \equiv (\mathrm{Tr}[P^\sigma] + 1)\,(\mathrm{Tr}[P^\sigma] + 1 + 2\sigma i)\,(\mathrm{Tr}[P^\sigma] + 1 - 2\sigma i),$$

Application of CL to SU(3) PLM (1/3)

Wrong convergence when only gauge cooling is applied — slow decay

$\beta = 0.5i,\ \kappa = 1,\ \mu = 0.5$

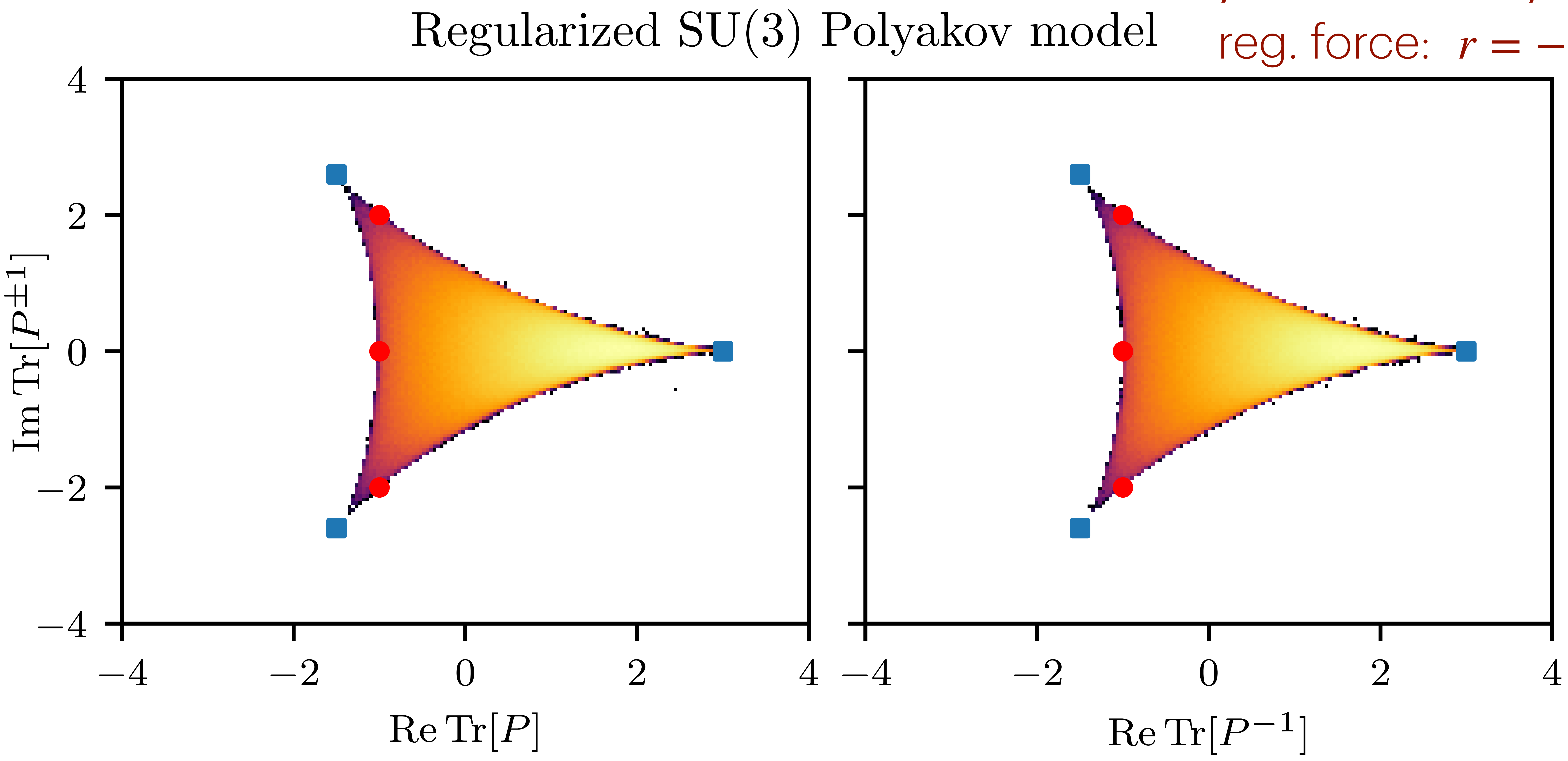


Application of CL to SU(3) PLM (2/3)

Compact/sharp density when regularization is applied — correct convergence

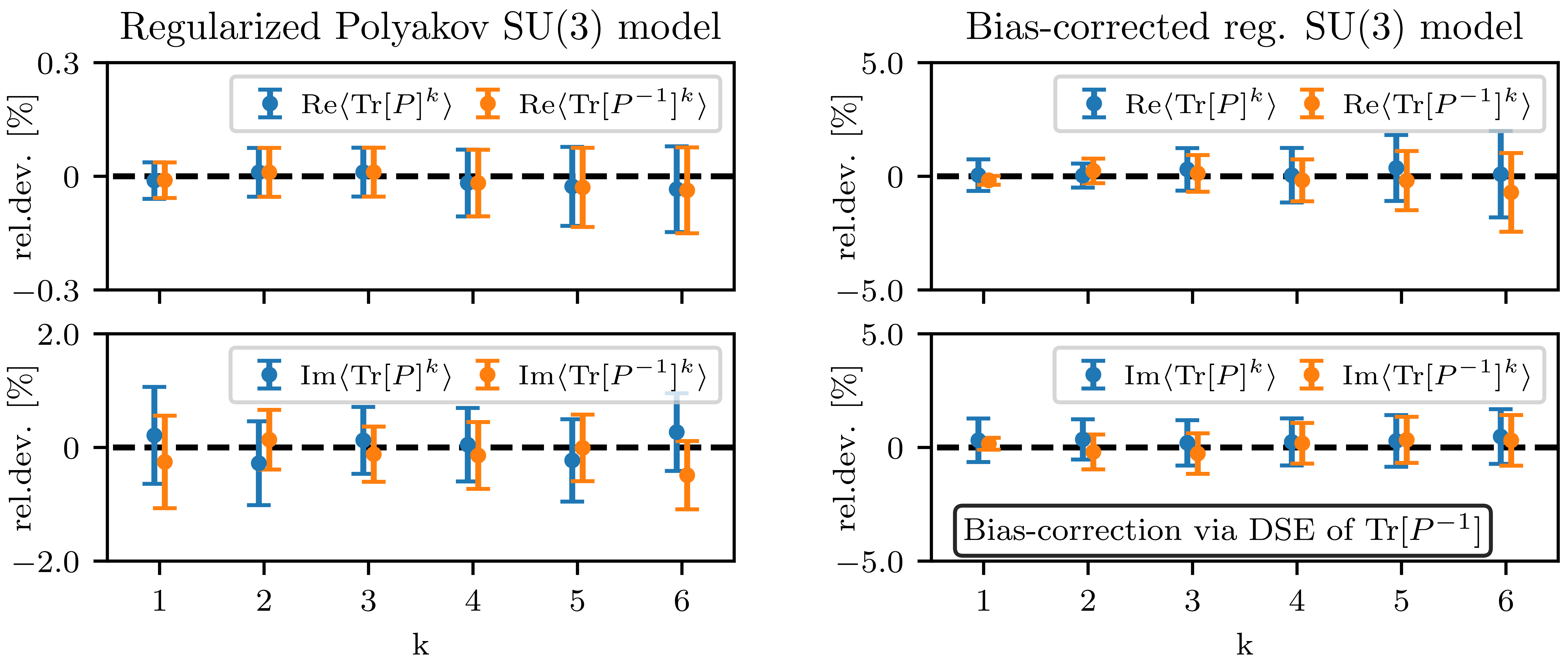
$\beta = 0.5i, \kappa = 1, \mu = 0.5$

reg. force: $r = -25$



Application of CL to SU(3) PLM (3/3)

Extraction of expectation values for original model



Conclusion

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

Ideas / work in progress:

- We develop a mathematical connection between thimbles and CL that allows us to **design kernel transformations** that admit similar Lefschetz thimbles
- Restricting the 'sampling space' for CL with prior information from Dyson-Schwinger equations
- Conceptional: find a mathematical formulation of the criterion of correctness in terms of thimbles

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 issues by regularizing the weight function:**
    - Design regularizations to obtain a **compact thimble structure**
    - We obtain **corrections from <u>prior knowledge</u>** using Dyson Schwinger equations

That's the key word for the next talk

→ Solution to the complex cosine model and the SU(N) 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!

Backup: Translating back to SU(N)

Why do we even test regularizations for SU(2)?

- The translation is straightforward but there are obvious and subtle differences
  → we want to apply methods to actual gauge field theories

- **Some important aspects:**

  1. Lefschetz thimbles are gauge-dependent, this leads to a manifold of thimbles for each stat. point
  2. Gauge cooling does not fully eliminate complexified gauge freedom
  3. Gauge freedom does not…

     - … map the Polyakov chain to a one-link model
     - … reduce the Haar measure as it does not affect the SU(2) symmetry