When Langevin met Lefschetz

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Complex actions

complex action problem

$$Z = \int dx\, e^{-S(x)} \qquad\qquad S(x) \in \mathbb{C}$$

explore the complex plane/complexified configuration space

today: two approaches

- complex Langevin dynamics
- Lefschetz thimbles

Cristoforetti, Di Renzo, Mukherjee, Scorzato

Kikukawa et al

relation?

Outline

three slightly disconnected observations:

- complex-mass model: distributions

  GA, PG & ES 1306.3075 (Annals Phys) GA 1308.4811 (PRD)

- finite-density inspired models, log det problem

- gauge cooling

as part of a joint effort with Nucu Stamatescu, Erhard Seiler, Denes Sexty

and Pietro Giudice, Jan Pawlowski

and for this talk in particular Lorenzo Bongiovanni

also correspondence with Gerald Dunne and Mithat Unsal

Langevin versus Lefschetz

Langevin dynamics:

zero-dimensional example
complex action $S(z)$

- $\dot{z} = -\partial_z S(z) + \eta \qquad z = x + iy$
- associated Fokker-Planck equation

$$\dot{P}(x,y;t) = [\partial_x(\partial_x + \mathrm{Re}\,\partial_z S(z)) + \partial_y \mathrm{Im}\,\partial_z S(z)]P(x,y;t)$$

- (equilibrium) distribution in complex plane: $P(x,y)$
- observables

$$\langle O(x+iy)\rangle = \frac{\int dxdy\, P(x,y) O(x+iy)}{\int dxdy\, P(x,y)}$$

- $P(x,y)$ real and non-negative: no sign problem
- criteria for correctness

Langevin versus Lefschetz

Lefschetz thimble:

zero-dimensional example
complex action $S(z)$

- critical points z_k where $\partial_z S(z) = 0$
- thimbles: $\mathrm{Im}\, S =$ cst, stable $\mathcal{J}_k$ and unstable $\mathcal{K}_k$
- integrate over stable thimbles

$$Z = \sum_k m_k e^{-i\mathrm{Im}\, S(z_k)} \int_{\mathcal{J}_k} dz\, e^{-\mathrm{Re}\, S(z)}$$

$$= \sum_k m_k e^{-i\mathrm{Im}\, S(z_k)} \int ds\, z'(s) e^{-\mathrm{Re}\, S(z(s))}$$

- residual sign problem: complex Jacobian $J(s) = z'(s)$
- global sign problem: phases $e^{-i\mathrm{Im}\, S(z_k)}$

Langevin versus Lefschetz

- Langevin

$$\langle O(z)\rangle = \frac{\int dxdy\, P(x,y) O(x+iy)}{\int dxdy\, P(x,y)}$$

- Lefschetz

$$\langle O(z)\rangle = \frac{\sum_k m_k e^{-i\mathrm{Im}\, S(z_k)} \int_{\mathcal{J}_k} dz\, e^{-\mathrm{Re}\, S(z)} O(z)}{\sum_k m_k e^{-i\mathrm{Im}\, S(z_k)} \int_{\mathcal{J}_k} dz\, e^{-\mathrm{Re}\, S(z)}}$$

- two- versus one-dimensional
- real versus residual/global phases

relation?

Quartic model

$$Z = \int_{-\infty}^{\infty} dx\, e^{-S} \qquad\qquad S(x) = \frac{\sigma}{2}x^2 + \frac{\lambda}{4}x^4$$

complex mass parameter $\sigma = A + iB$, $\lambda \in \mathbb{R}$

often used toy model Ambjorn & Yang 85, Klauder & Petersen 85, Okamoto et al 89, Duncan & Niedermaier 12

essentially analytical proof*: GA, PG & ES 13

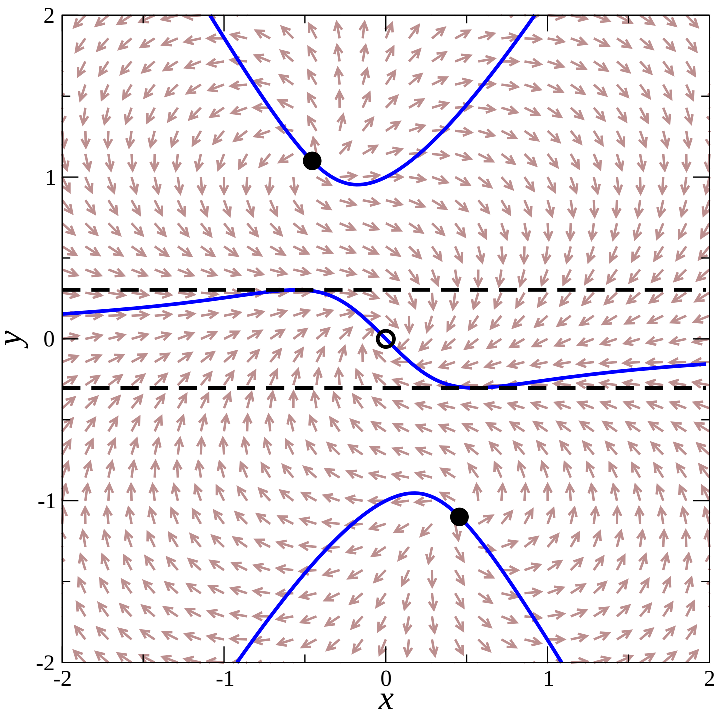
- CL gives correct result for all observables $\langle x^n \rangle$ provided that $A > 0$ and $A^2 > B^2/3$
- based on properties of the distribution $P(x, y)$
- follows from classical flow or directly from FPE

* GA, ES, IOS 09, + FJ 11

Quartic model

classical flow

$(A = B = 1)$



- determine where drift $K_{\rm I} = -{\rm Im}\,\partial_z S(z)$ vanishes (blue lines)
- at the extrema: impenetrable barrier (for real noise)
- distribution localised between dashed lines

Quartic model

from Fokker-Planck equation:

- FPE can be written as $\dot{P} = \nabla \cdot \vec{J}$
- vanishing charge, with $\partial_y Q(y) = 0$,

$$Q(y) = \int dx\, J_y(x,y) = \int dx\, K_{\mathrm{I}}\,(x,y) P(x,y) = 0$$

since $P(x,y) \geq 0$:

- when K_{I} has definite sign, $P(x,y)$ has to vanish

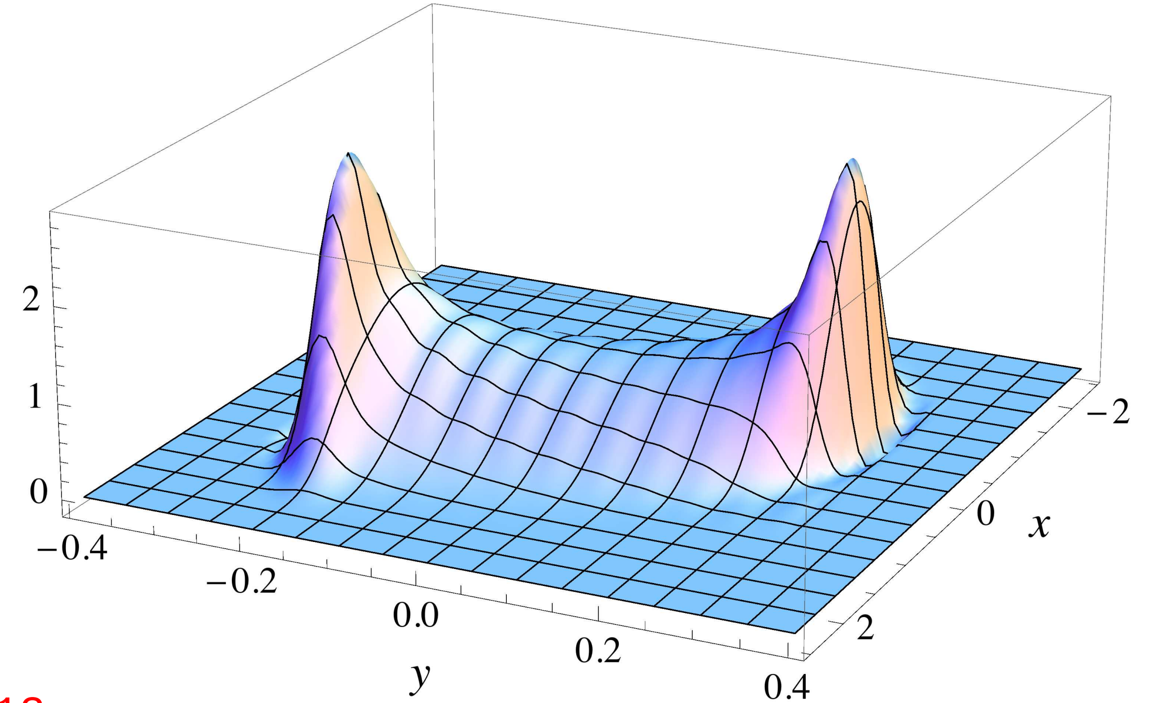
stripes: $$y_-^2 < y^2 < y_+^2$$

with

$$y_\pm^2 = \frac{1}{2\lambda}\left(A \pm \sqrt{A^2 - B^2/3}\right)$$

Quartic model

- numerical solution of FPE for $P(x, y)$
  following Duncan & Niedermaier 12
- distribution is localised in a strip around real axis
- $|y| < y_-$ with $y_- = 0.3029$ for $A = B = 1$



GA, PG & ES 13

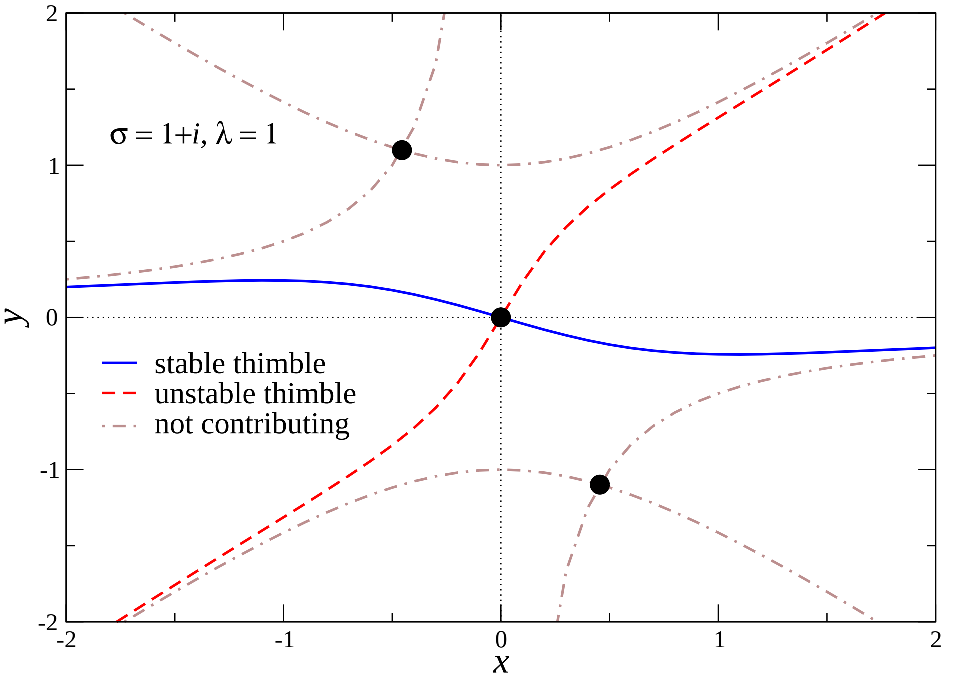
Quartic model

relation to Lefschetz thimbles

GA 13

- critical points:

$$z_0 = 0$$
$$z_\pm = \pm i\sqrt{\sigma/\lambda}$$



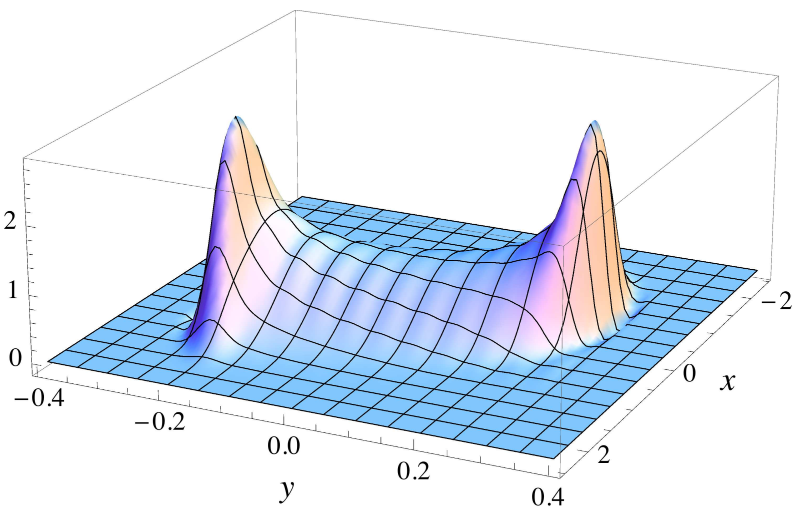
- thimbles can be computed analytically

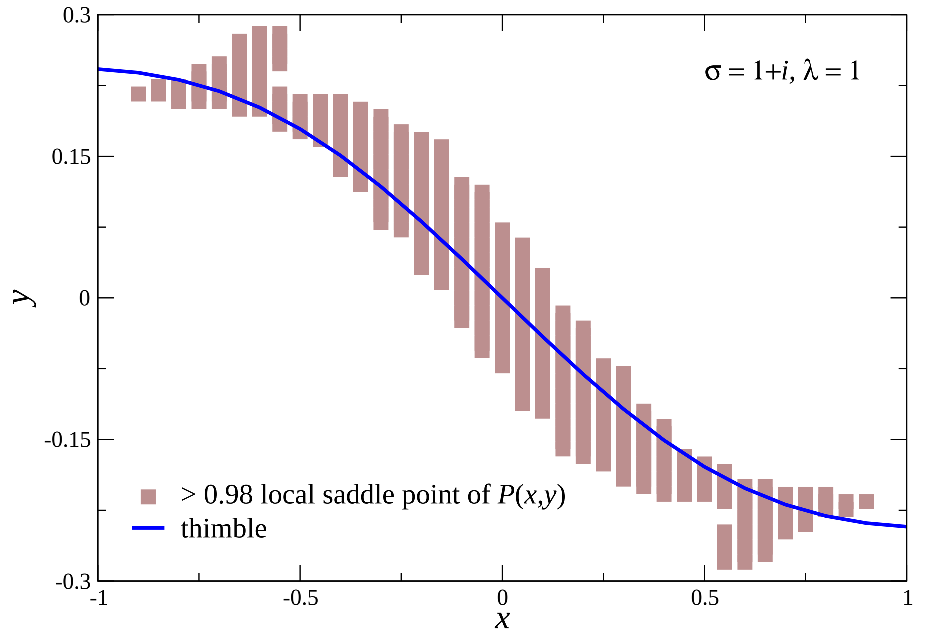
$$\mathrm{Im}\, S(z_0) = 0$$
$$\mathrm{Im}\, S(z_\pm) = -AB/2\lambda$$

- for $A > 0$: only 1 thimble contributes
- integrating along thimble gives correct result, with inclusion of complex Jacobian

Quartic model

compare thimble and FP distribution $P(x, y)$



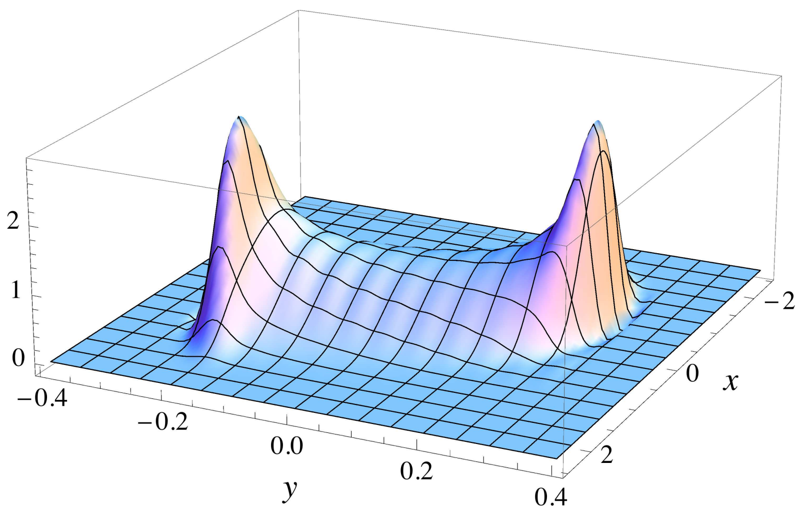


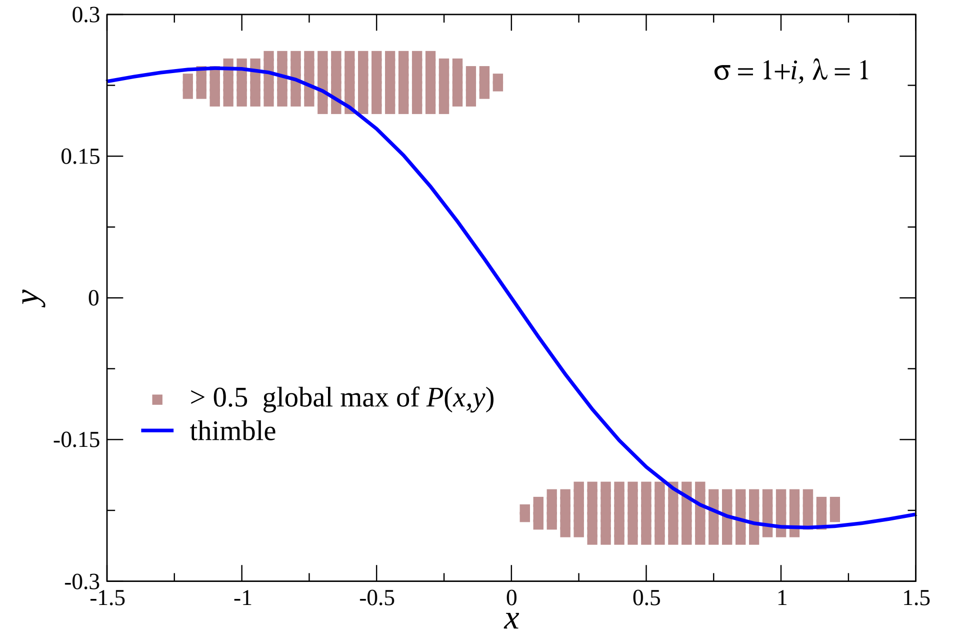
- thimble and $P(x, y)$ follow each other
- however, weight distribution quite different

intriguing result: CLE finds the thimble – is this generic?

Quartic model

compare thimble and FP distribution $P(x, y)$





- thimble and $P(x, y)$ follow each other
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intriguing result: CLE finds the thimble – is this generic?

U(1) model at nonzero density

U(1) one-link model for finite density GA & IOS 08

$$Z = \int dU\, e^{-S_B} \det M$$
$$= \int_{-\pi}^{\pi} dx\, e^{\beta \cos x} [1 + \kappa \cos(x - i\mu)]$$

- when $\kappa < 1$: correct results for real β and all μ
- smooth deformation of distributions as μ is increased

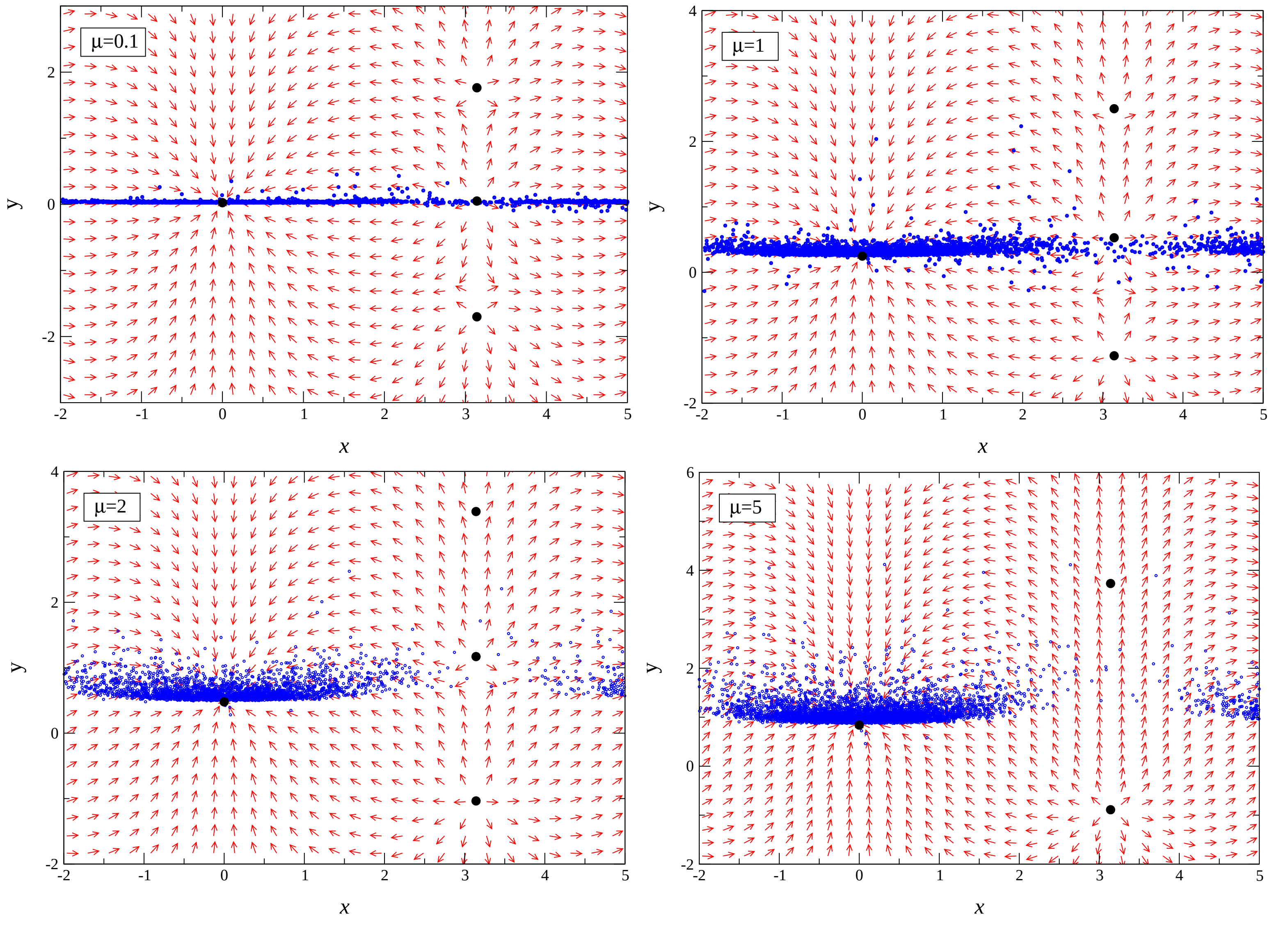
- when $\kappa > 1$: real sign problem already at $\mu = 0$
- presence of $\log \det$ of interest for CLE and thimbles

Mollgaard & Splittorff 13, Seiler et al 14

U(1) model at nonzero density

distribution in complex plane

GA & IOS 08



U(1) model at nonzero density

relation with thimble $S(z) = -\beta \cos z - \ln[1 + \kappa \cos(z - i\mu)]$

new feature:

- action not holomorphic
- diverging drift when $1 + \kappa \cos(z - i\mu) = 0$
- $\mathrm{Im}\, S$ jumps

U(1) model at nonzero density

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- $\mathrm{Im}\, S$ jumps

some thimbles easily found: $z = iy$ and $z = \pm\pi + iy$

U(1) model at nonzero density

relation with thimble $S(z) = -\beta \cos z - \ln[1 + \kappa \cos(z - i\mu)]$

new feature:

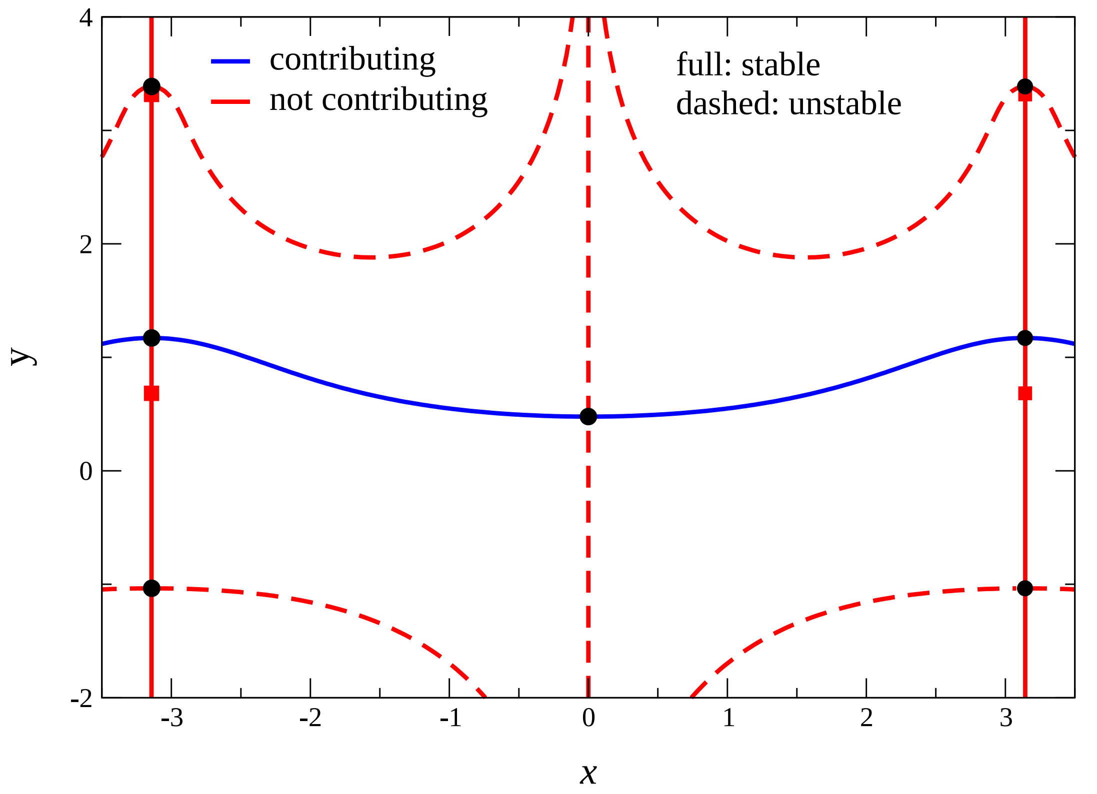
- action not holomorphic
- diverging drift when $1 + \kappa \cos(z - i\mu) = 0$
- $\mathrm{Im}\, S$ jumps

nature of thimbles depends on κ

- $\kappa < 1$:
  - action real when $\mu = 0$
  - drift diverges on $x = \pm\pi$ axis
- $\kappa > 1$:
  - action complex even when $\mu = 0$ – sign problem
  - drift diverges away from $x = \pm\pi$ axis

U(1) model at nonzero density

$\kappa = 0.25 < 1$
$\beta = 1$
$\mu = 2$

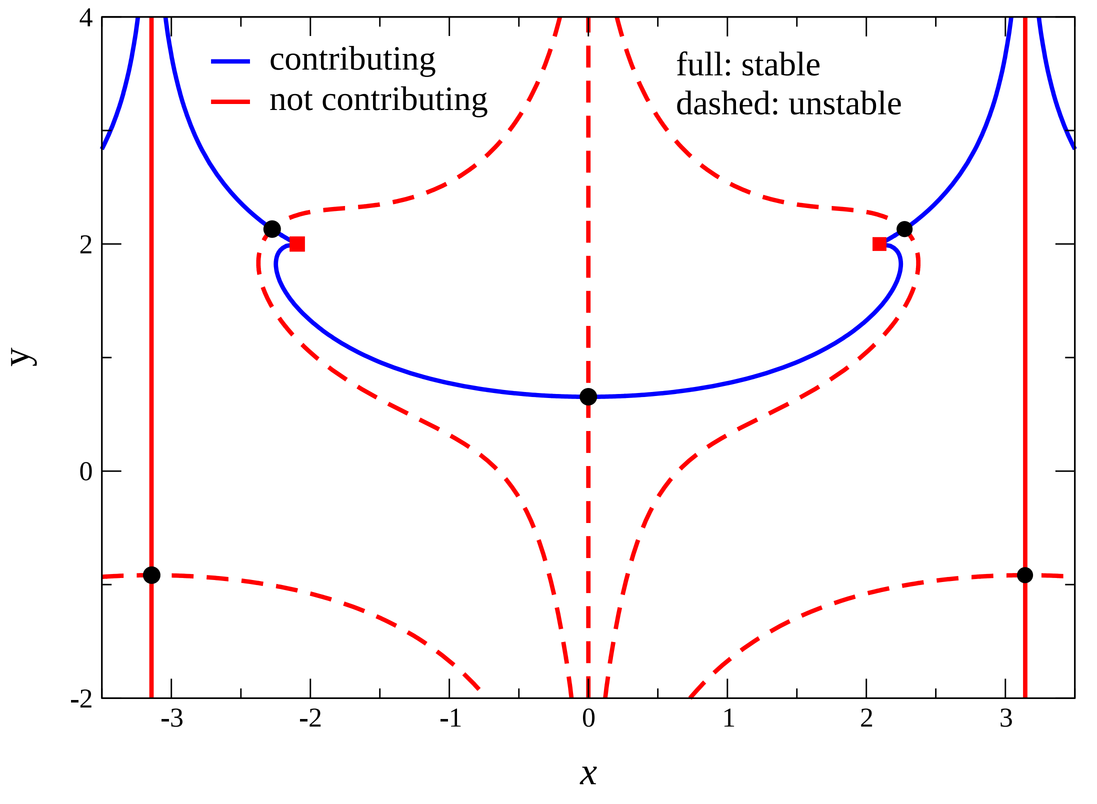


- circles: critical points
- boxes: drift diverges, $\mathrm{Im}\, S$ jumps by π, flow changes direction

one stable contributing thimble (blue)

U(1) model at nonzero density

$\kappa = 2 > 1$
$\beta = 1$
$\mu = 2$

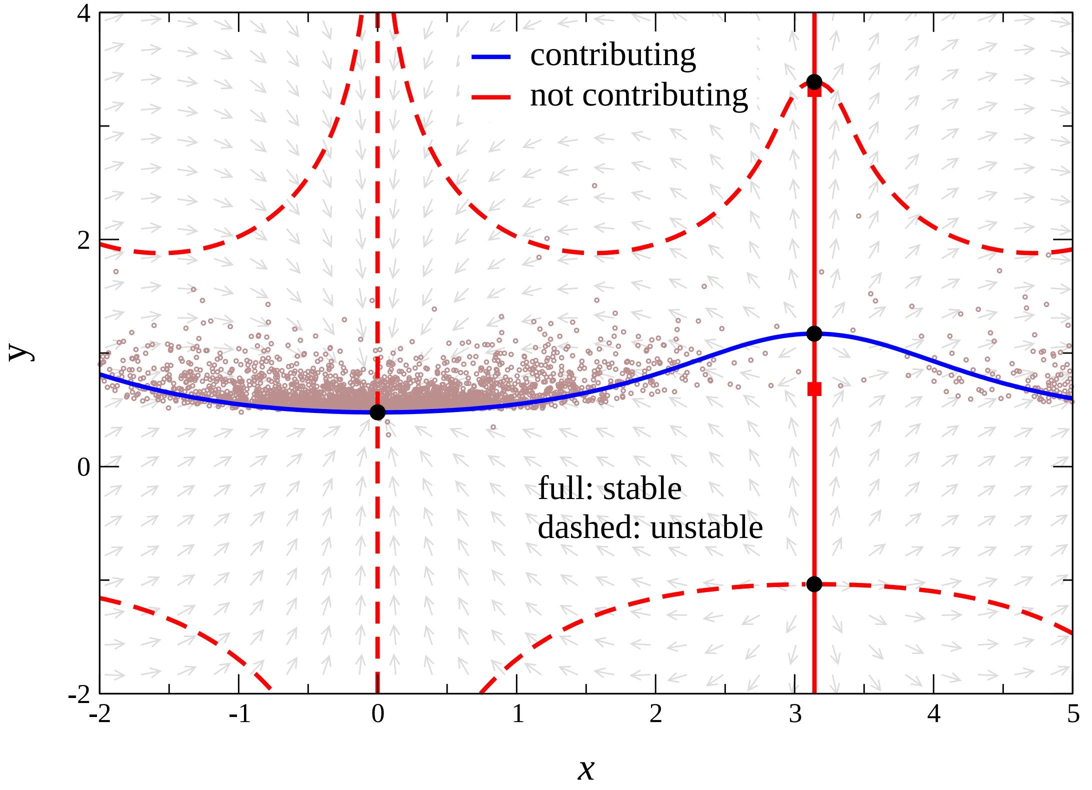


- circles: critical points
- boxes: drift diverges, $\mathrm{Im}\, S$ jumps by amount depending on parameters, flow changes direction

two stable thimbles (blue), global phase problem

U(1) model at nonzero density

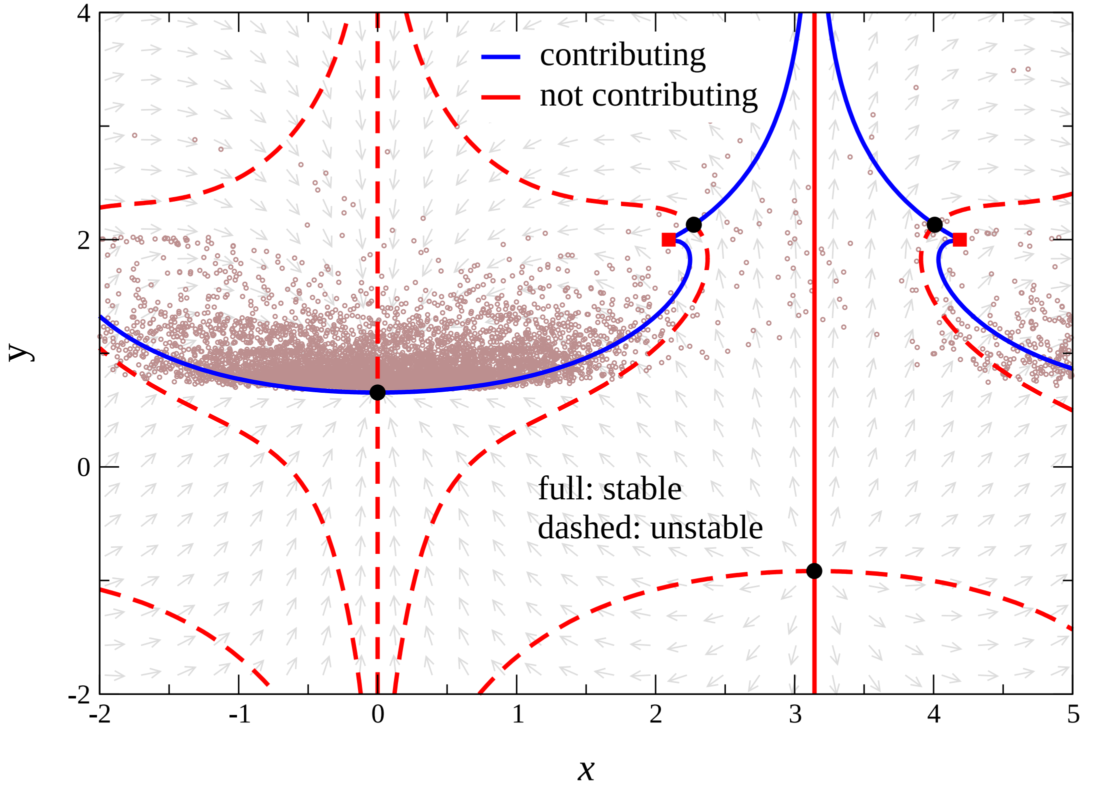
$\kappa = 0.25 < 1$
$\beta = 1$
$\mu = 2$



- comparison with scatter plots of CLE from 2008 paper
- $P(x, y)$ and thimble find each other
- CLE and single thimble both give correct result

U(1) model at nonzero density

$\kappa = 2 > 1$
$\beta = 1$
$\mu = 2$



- comparison with scatter plots of CLE when $\kappa > 1$
- CLE gives wrong result
- both stable thimbles contribute, global phase problem

U(1) model at nonzero density

diverging drift, action not holomorphic

- thimbles end at singular points
- $\mathrm{Im}\, S$ jumps
- potential for global phase problems

in this model

when $\kappa < 1$:

- no sign problem when $\mu = 0$
- at nonzero μ, both CLE and thimble are effective

when $\kappa > 1$:

- real sign problem when $\mu = 0$
- both CLE and thimbles are ineffective

SU(2) model

SU(2) one-link model with complex β

$$Z = \int dU\, e^{-S(U)} \qquad\qquad S(U) = -\frac{\beta}{2}\mathrm{Tr}\, U$$

can be solved with CL in different ways:

- fully 'gauge fixed': diagonalise and include reduced Haar measure

$$Z = \int_{-\pi}^{\pi} dx\, \sin^2 x\, e^{\beta \cos x} = \int_{-\pi}^{\pi} dx\, e^{-S(x)}$$

- diagonalise after each CL update `Berges & Sexty 08`
- group dynamics with gauge cooling `ES, DS & IOS 13`

$$U' = \Omega R U \Omega^{-1} \qquad\qquad R = e^{i\sigma_a(\epsilon K_a + \sqrt{\epsilon}\eta_a)}$$

SU(2) model: gauge fixed

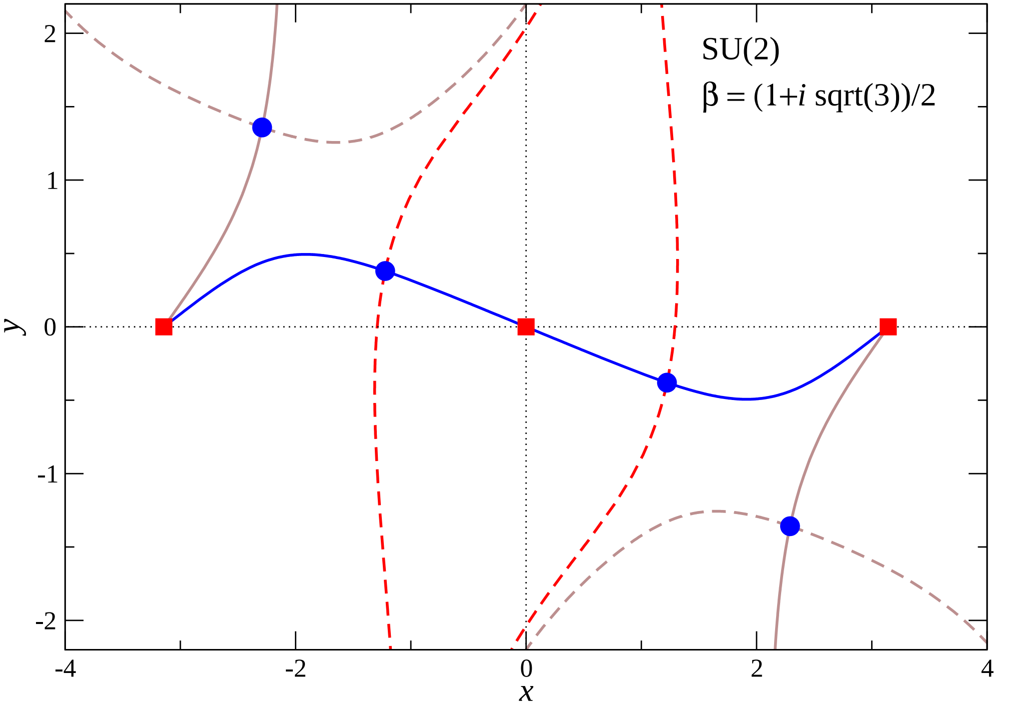
first approach: fully gauge fixed

$$Z = \int_{-\pi}^{\pi} dx\, e^{-S(x)} \qquad S(x) = -\beta \cos x - \ln \sin^2 x$$

- drift $\partial_z S(z) = \beta \sin z - 2 \cot z$ has poles at $z = 0, \pm\pi$
- fixed points given by

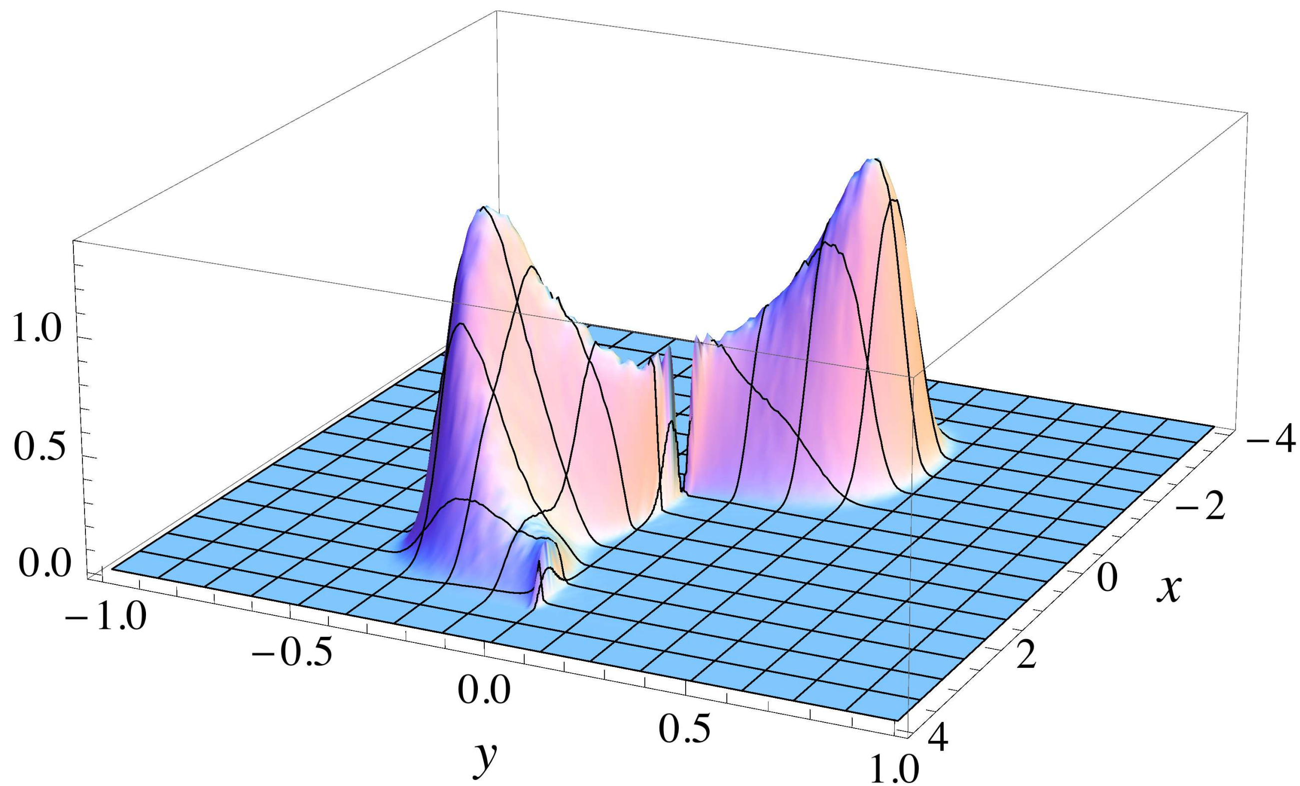
$$\cos z = -\frac{1}{\beta}(1 \pm \sqrt{1+\beta^2})$$

- thimbles easily found



SU(2) model: gauge fixed

comparison between Langevin and Lefschetz

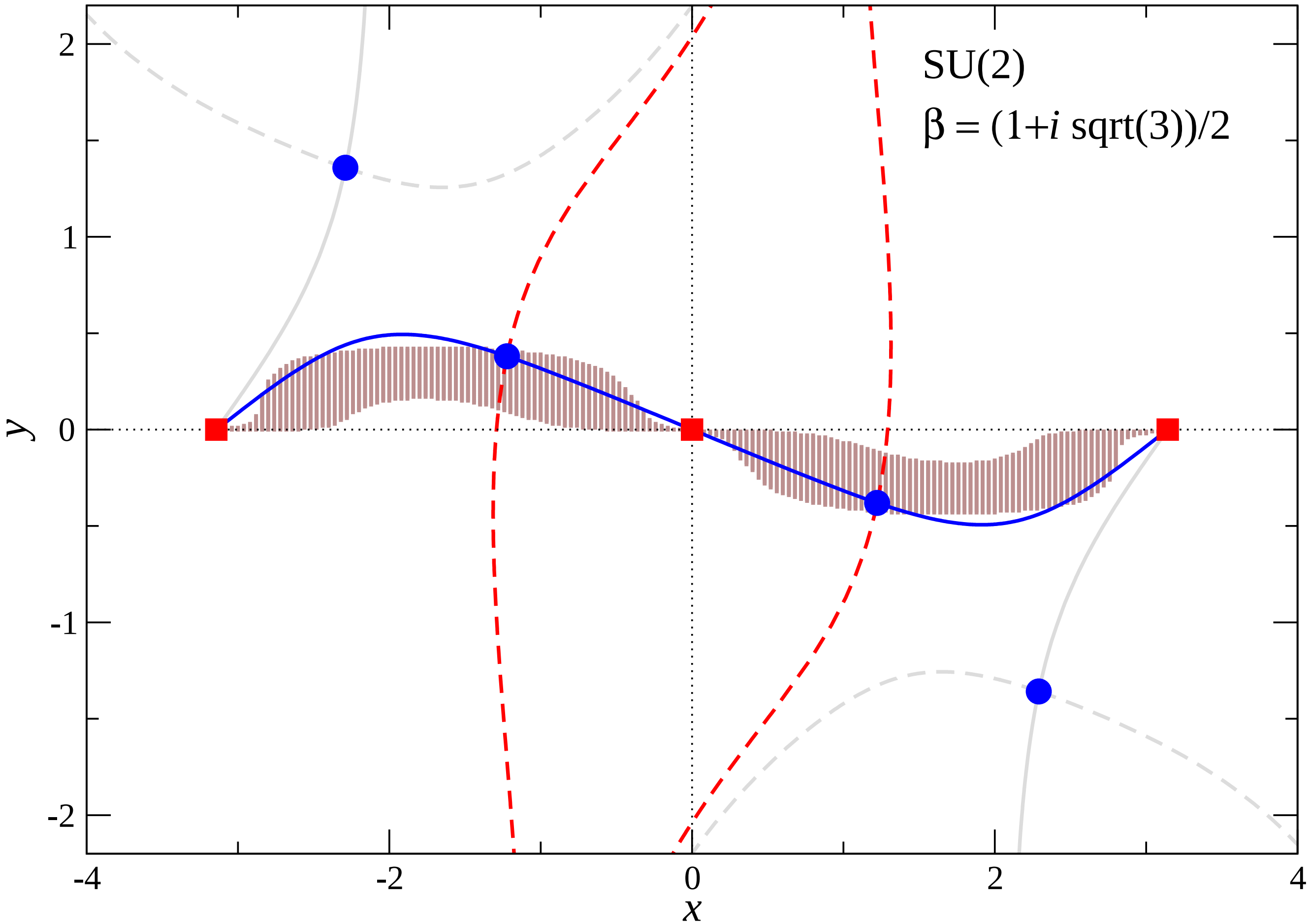


CL histogram in xy plane

- well-localised, correct results obtained

SU(2) model: gauge fixed

comparison between Langevin and Lefschetz

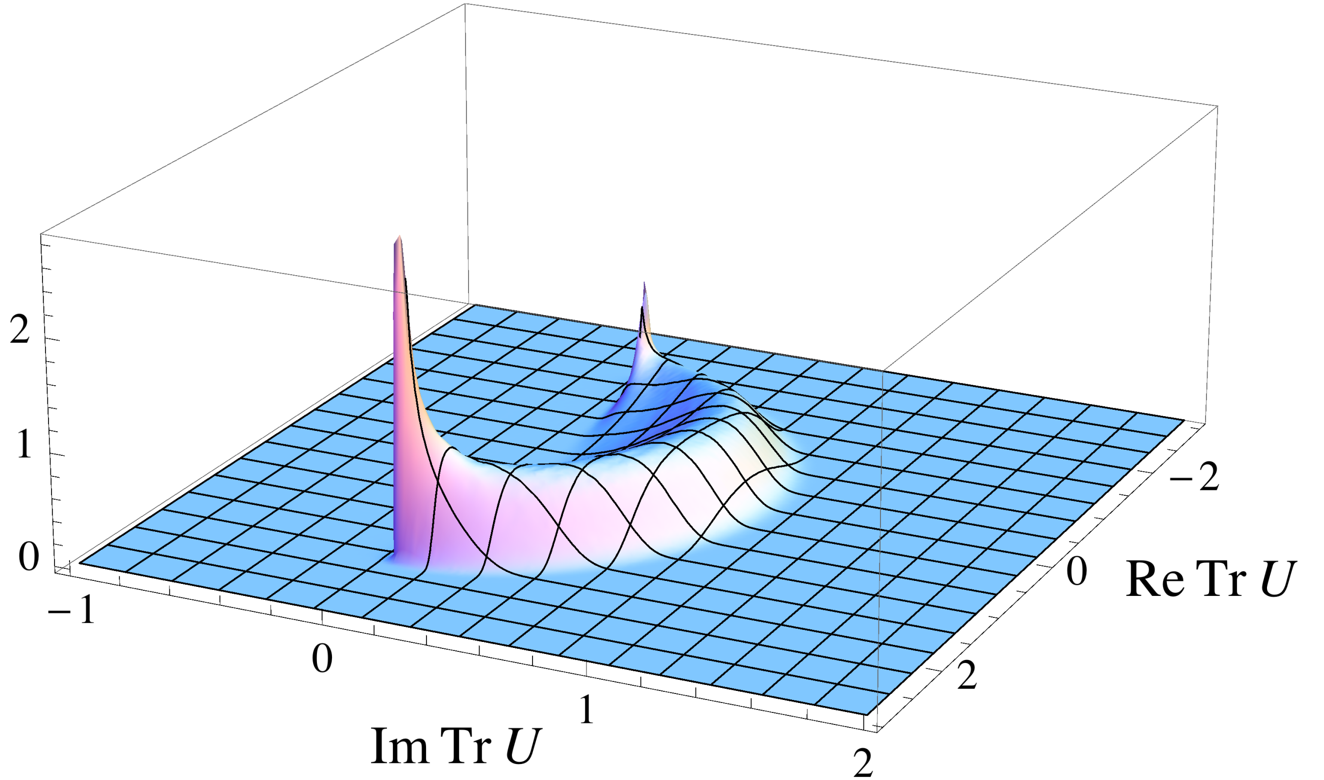


CL distribution and thimbles follow each other

SU(2) model

comparison between Langevin and Lefschetz

- use gauge invariant variable $\mathrm{Tr}\, U$

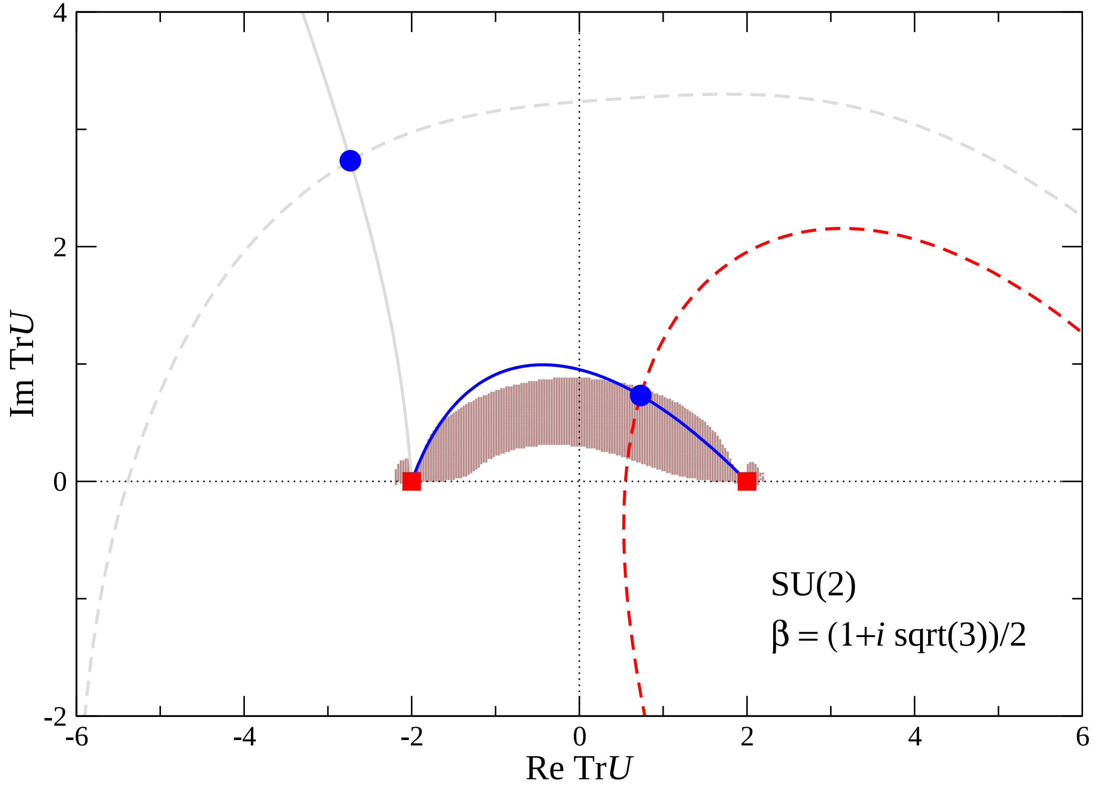


CL histogram in $\mathrm{Tr}\, U$ plane

SU(2) model

comparison between Langevin and Lefschetz

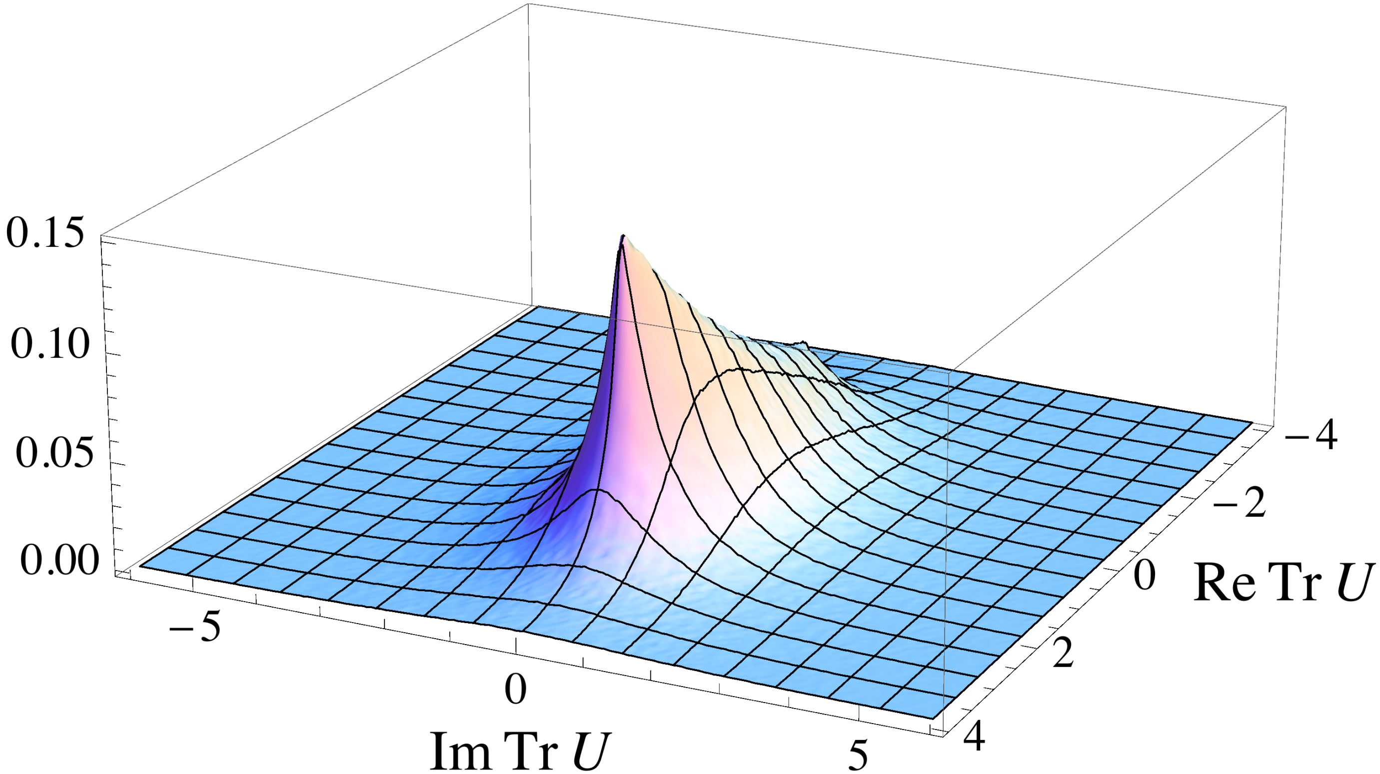
- use gauge invariant variable $\mathrm{Tr}\, U$
- map thimbles into $\mathrm{Tr}\, U$ plane
- comparison with CL histogram for $\mathrm{Tr}\, U$



SU(2) model: gauge cooling

use group dynamics and gauge cooling

- distribution in $\mathrm{Tr}\, U$ plane

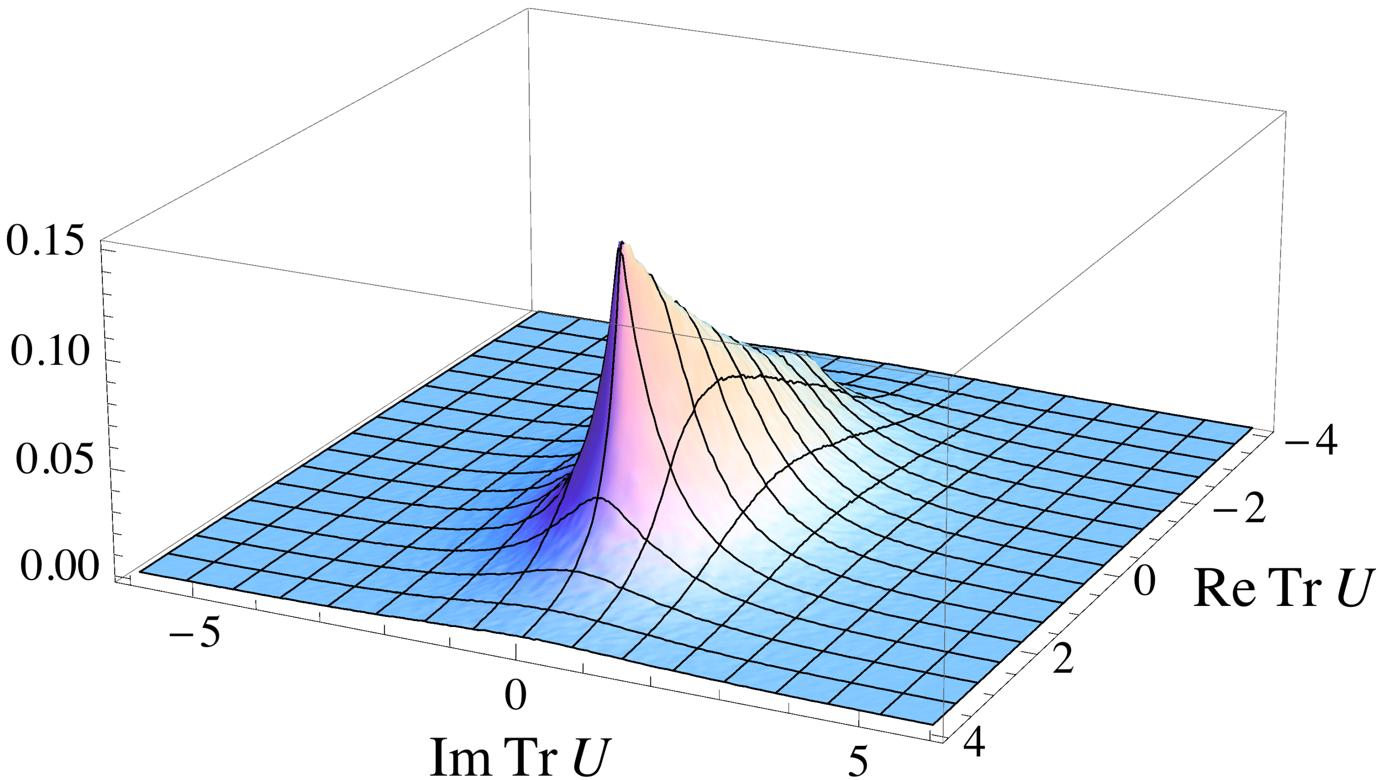


- number of cooling steps: 0
- wide distribution, wrong results

SU(2) model: gauge cooling

use group dynamics and gauge cooling

- distribution in $\mathrm{Tr}\,U$ plane

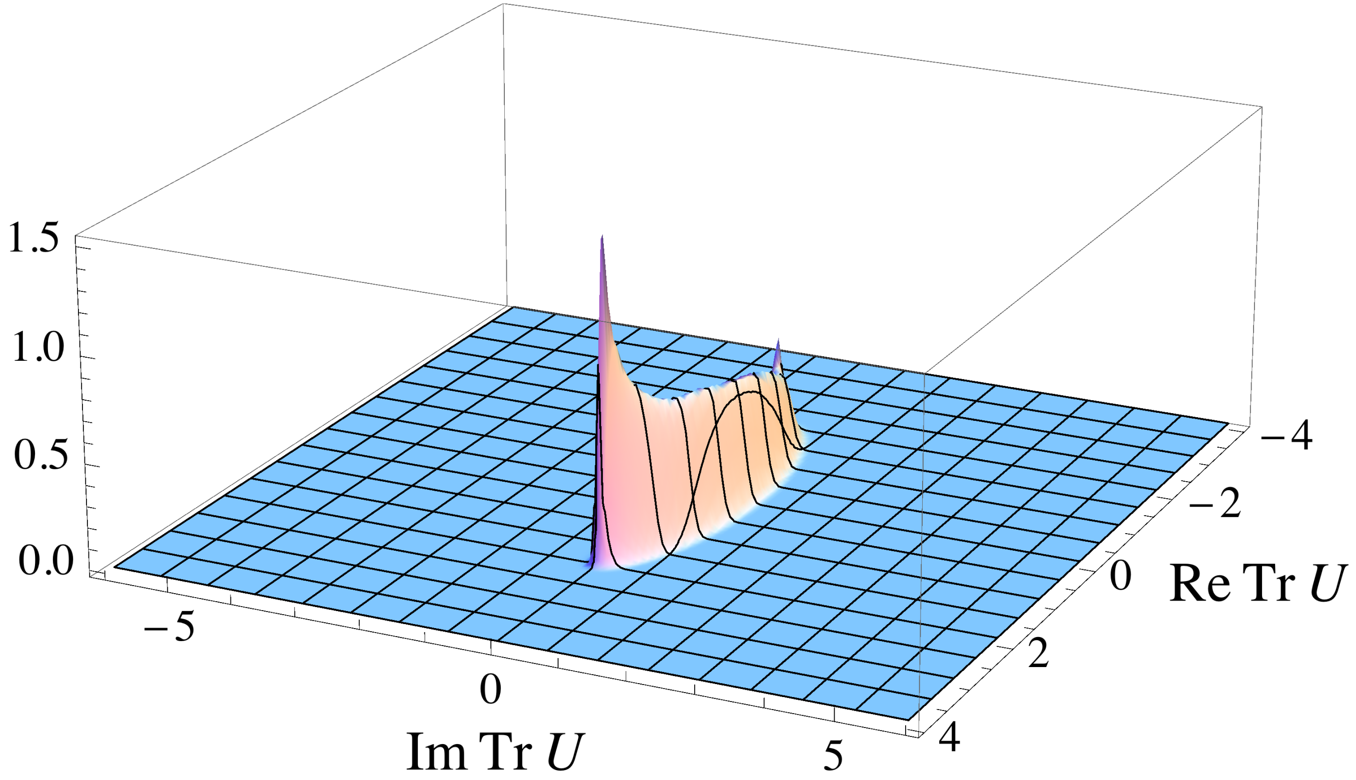


- number of cooling steps: 1
- wide distribution, wrong results

SU(2) model: gauge cooling

use group dynamics and gauge cooling

- distribution in $\mathrm{Tr}\, U$ plane

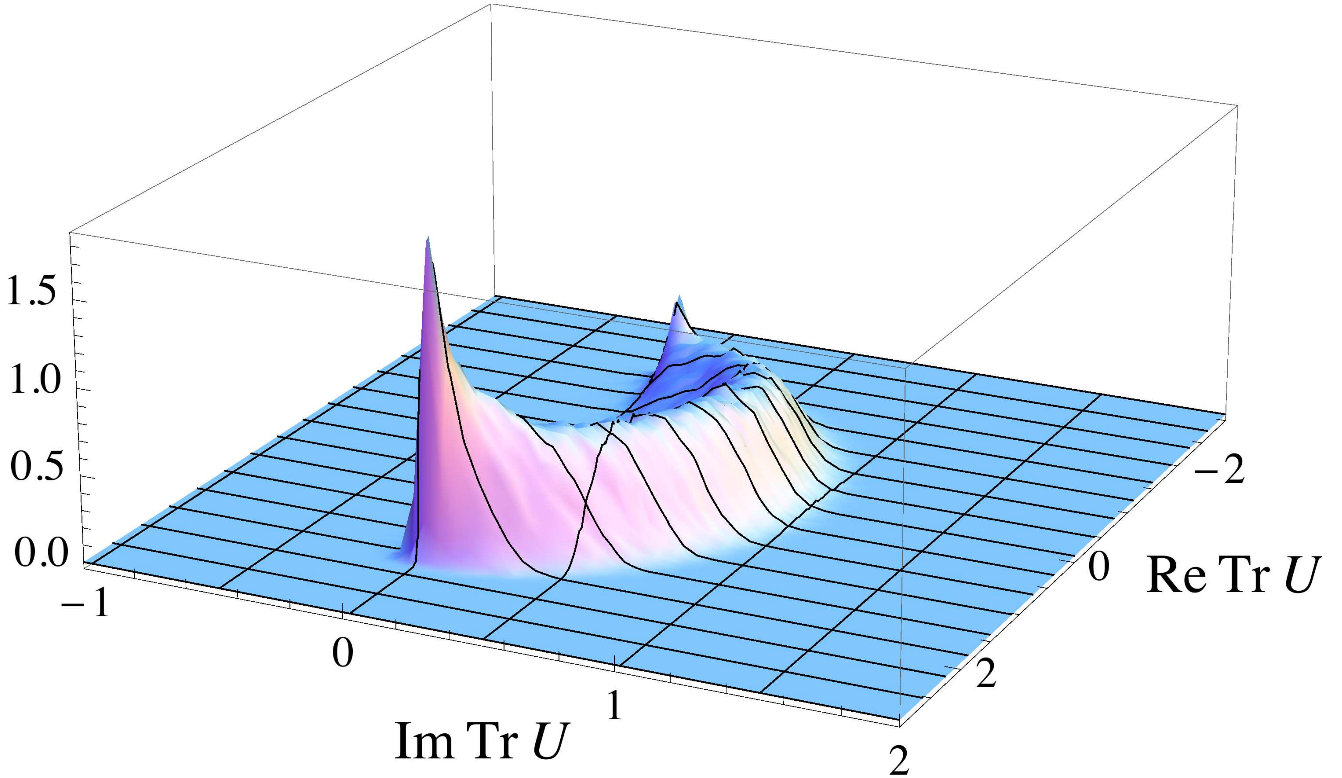


- number of cooling steps: 2
- narrow distribution, correct results

SU(2) model: gauge cooling

use group dynamics and gauge cooling

- distribution in $\mathrm{Tr}\,U$ plane

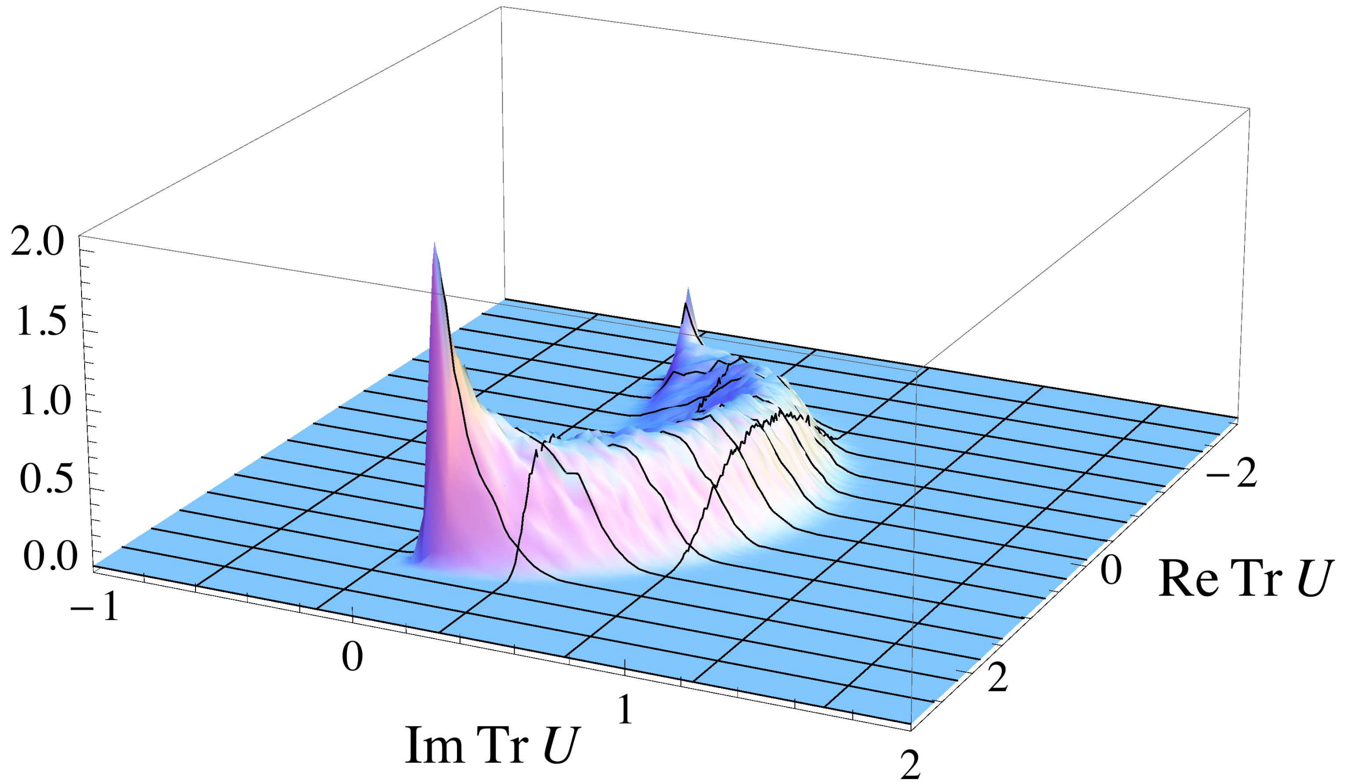


- number of cooling steps: 4
- narrow distribution, correct results

SU(2) model: gauge cooling

use group dynamics and gauge cooling

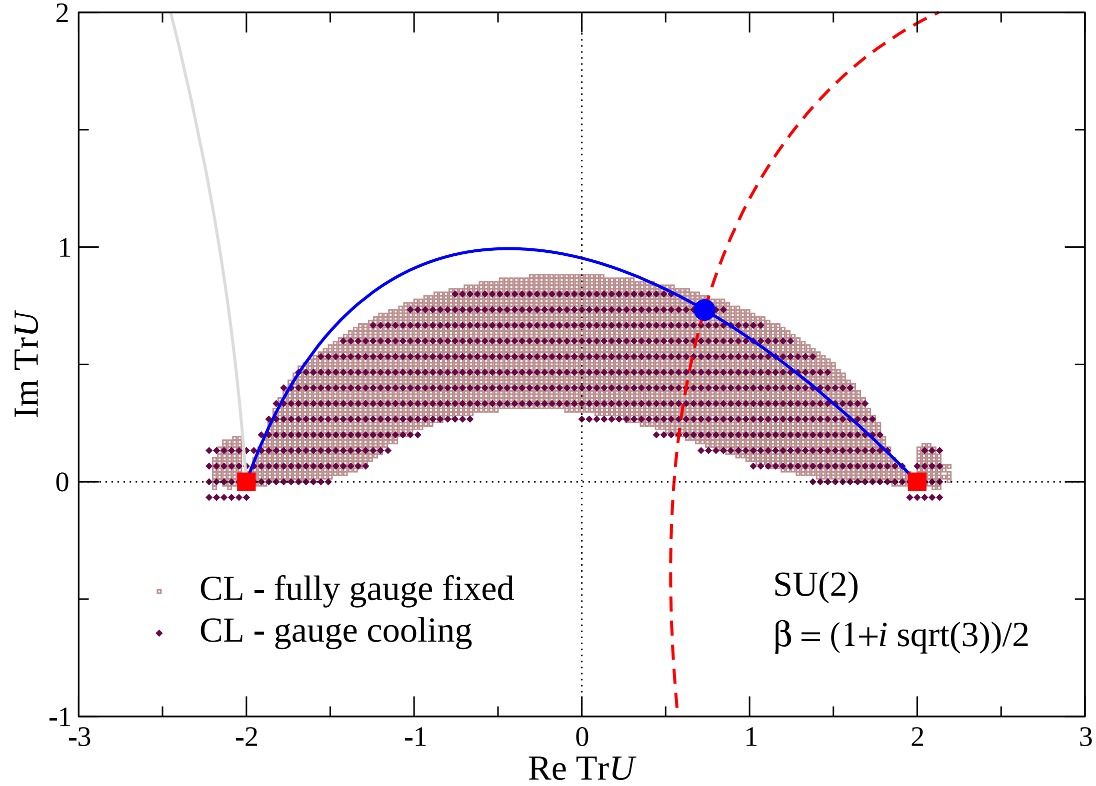
- distribution in $\mathrm{Tr}\, U$ plane



- number of cooling steps: 6
- narrow distribution, correct results

SU(2) model: gauge cooling

use group dynamics and gauge cooling



- gauge cooling and full gauge fixing yield the same distributions
- CL dynamics under control

SU(2) model

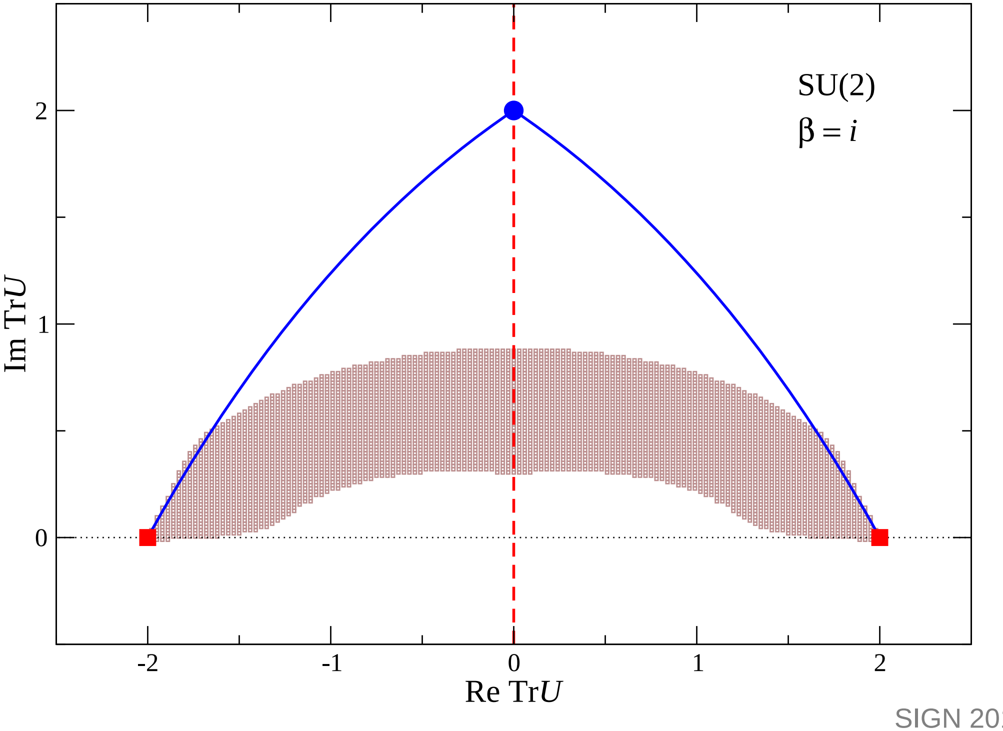
special case $\beta = i$ Berges & Sexty 08

- *degenerate* critical point at $\cos z = i$, $\partial_z^2 S(z) = 0$
- thimbles can be computed analytically

$$v(u) = \frac{1}{\tan u}\left(u \pm \sqrt{u^2 - (1-u^2)\tan^2 u}\right)$$

- in terms of
  $\frac{1}{2}\mathrm{Tr}\, U = \cos z$
  $= u + iv$

- CL distribution
  pinched by thimbles



Summary

observations in simple models:

- CL distribution and thimbles related
- CL samples ‘smeared’ distribution close to thimble
- since CL distribution is real: 1D $\rightarrow$ 2D is necessary
- log det problem depends on details of model (for both)

crisp relation between CL and thimble structure is lacking
only circumstantial