

Complex actions, complex Langevin and Lefschetz thimbles

Gert Aarts



Swansea University
Prifysgol Abertawe

Motivation

QCD partition function

at nonzero quark chemical potential

$$[\det D(\mu)]^* = \det D(-\mu^*)$$

- fermion determinant is complex
- straightforward importance sampling not possible
- sign problem

⇒ QCD phase diagram has not yet been determined non-perturbatively

Outline

- complex actions
- Langevin dynamics
- thimble dynamics
- Langevin versus Lefschetz
- summary

GA, Phys. Rev. D 88 (2013) 094501 (1308.4811)

GA, Lorenzo Bongiovanni, Erhard Seiler & Dénes Sexty, 1407.2090

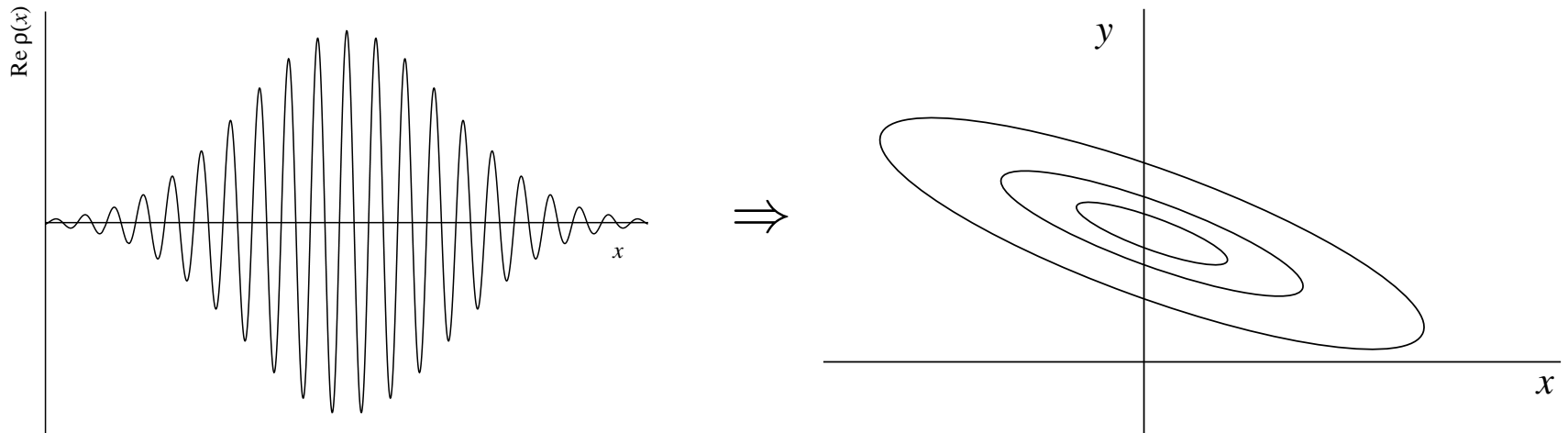
GA, Pietro Giudice & Erhard Seiler, Annals Phys. 337 (2013) 238
(1306.3075)

Complex actions

one degree of freedom: $Z = \int dx e^{-S(x)}$

complex holomorphic action $S(z) \in \mathbb{C}$

- numerical sign problem
- dominant configurations in the (path) integral?



- real and positive distribution $P(x, y)$?

Complex actions

various approaches relying on holomorphicity:
go into the complex plane

- saddle point/steepest descent: Lefschetz thimbles

Witten 10

Cristoforetti, Di Renzo, Mukherjee, Scorzato, (Schmidt) 12-14

Fujii, Honda, Kato, Kikukawa, Komatsu, Sano 13

Dunne, Unsal et al 12-14

...

- complex Langevin dynamics/stochastic quantisation

GA, Seiler, Sexty, Stamatescu,

James, Bongiovanni, Giudice, Jaeger, Attanasio

...

see talk by Dénes Sexty for progress in gauge theories

Complex Langevin dynamics

Langevin dynamics:

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

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

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

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

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

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

Lefschetz thimbles

generalised saddle point integration/steepest descent:

extend definition of path integral

Witten 10

- Chern-Simons theories
- mathematical foundation in Morse theory

formulation:

- find *all* stationary points z_k of holomorphic action $S(z)$
- paths of steepest descent: stable thimbles \mathcal{J}_k
- paths of steepest ascent: unstable thimbles \mathcal{K}_k
- $\text{Im } S(z)$ constant along thimble k

integrate over stable thimbles, with proper weighting

Lefschetz thimbles

generalised saddle point integration/steepest descent:

- integrate over stable thimbles

$$\begin{aligned} Z &= \sum_k m_k e^{-i\text{Im}S(z_k)} \int_{\mathcal{J}_k} dz e^{-\text{Re}S(z)} \\ &= \sum_k m_k e^{-i\text{Im}S(z_k)} \int ds z'(s) e^{-\text{Re}S(z(s))} \end{aligned}$$

- intersection numbers: $m_k = \langle C, \mathcal{K}_k \rangle$
(C = original contour, \mathcal{K}_k = unstable thimble)
- residual sign problem: complex Jacobian $J(s) = z'(s)$
- global sign problem: phases $e^{-i\text{Im}S(z_k)}$

Lefschetz thimbles

numerical Lefschetz approach

di Renzo et al 12

- find all saddle points/thimbles in field theory?
- integrate over dominant thimble \mathcal{J}_0 only

$$Z = e^{-i\text{Im}S(z_0)} \int_{\mathcal{J}_0} dz e^{-\text{Re}S(z)}$$

- motivated by universality
- no global sign problem
- residual sign problem remaining

validity?

- successful e.g. in interacting 4-dim Bose gas with $\mu \neq 0$

Langevin versus Lefschetz

two approaches in the complex plane:

- Langevin

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

- Lefschetz

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

- two- versus one-dimensional

- real versus residual/global phases

relation? validity? \Rightarrow simple models

Langevin versus Lefschetz



Quartic model

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

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

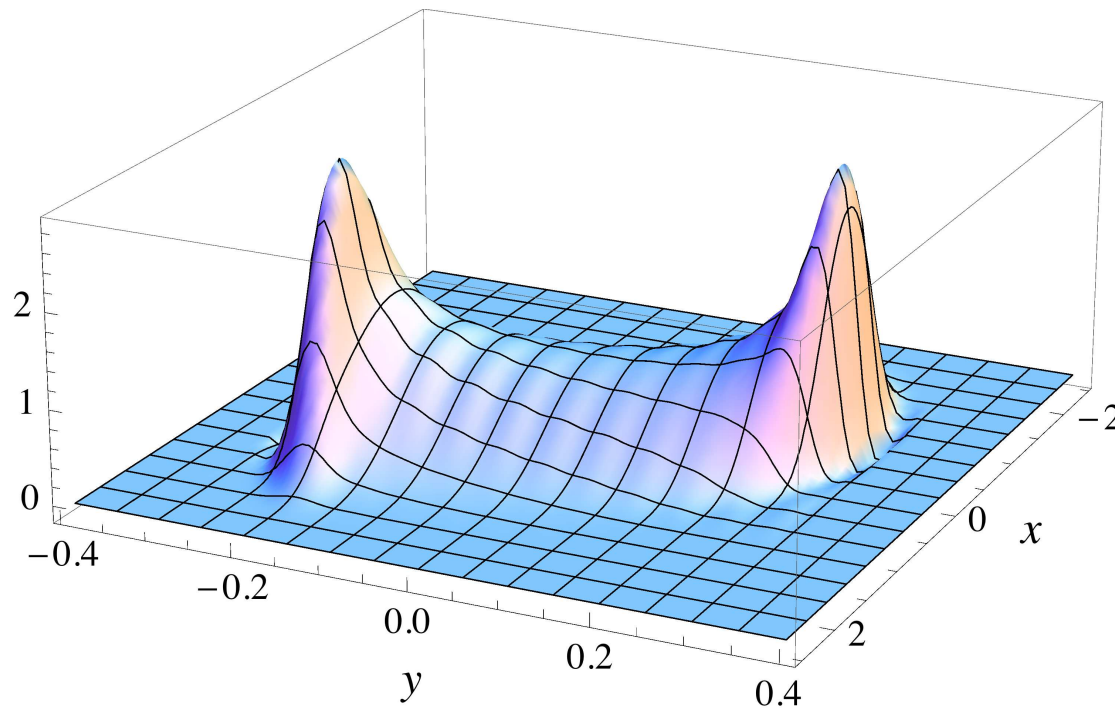
essentially analytical proof for CL*: GA, Giudice & Seiler 13

- 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, Seiler, Stamatescu 09 + James 11

Quartic model

- numerical solution of FPE for $P(x, y)$
- distribution is localised in a strip around real axis
- $P(x, y) = 0$ when $|y| > y_-$ with $y_- = 0.303$ for $\sigma = 1 + i$



Langevin versus Lefschetz

Lefschetz thimbles for quartic model

- critical points:

$$z_0 = 0$$

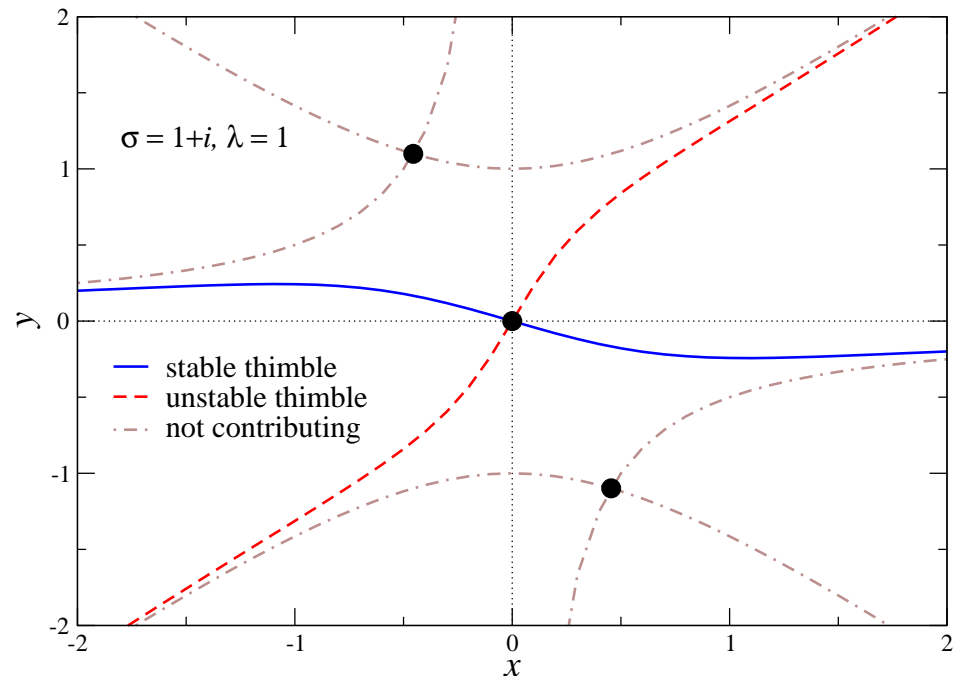
$$z_{\pm} = \pm i \sqrt{\sigma/\lambda}$$

- thimbles can be computed analytically

$$\text{Im}S(z_0) = 0$$

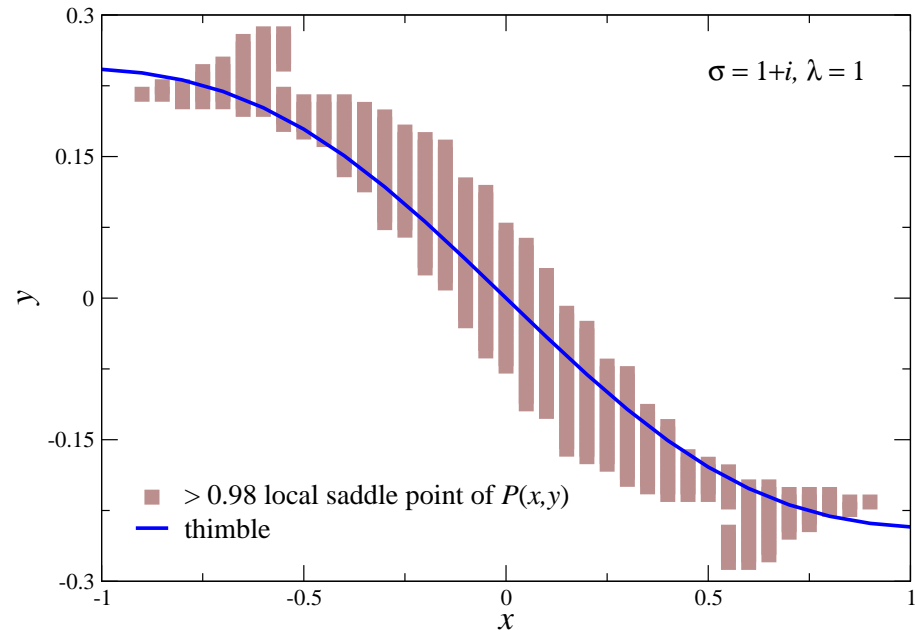
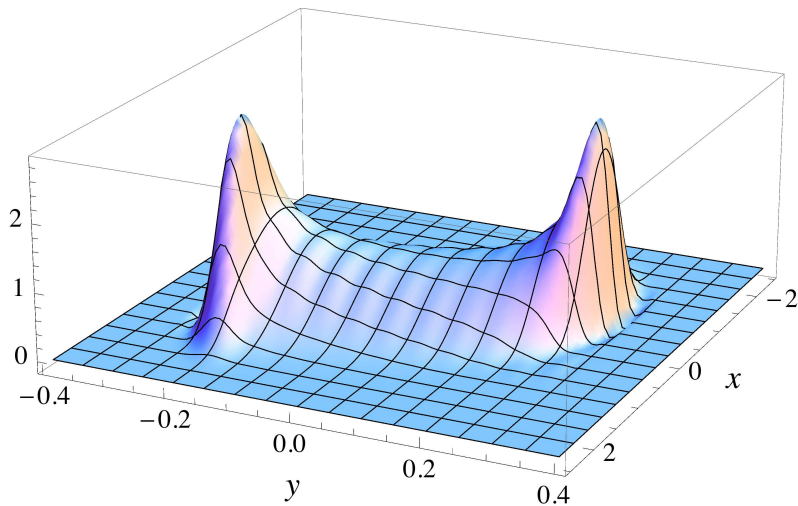
$$\text{Im}S(z_{\pm}) = -AB/2\lambda$$

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



Quartic model: thimbles

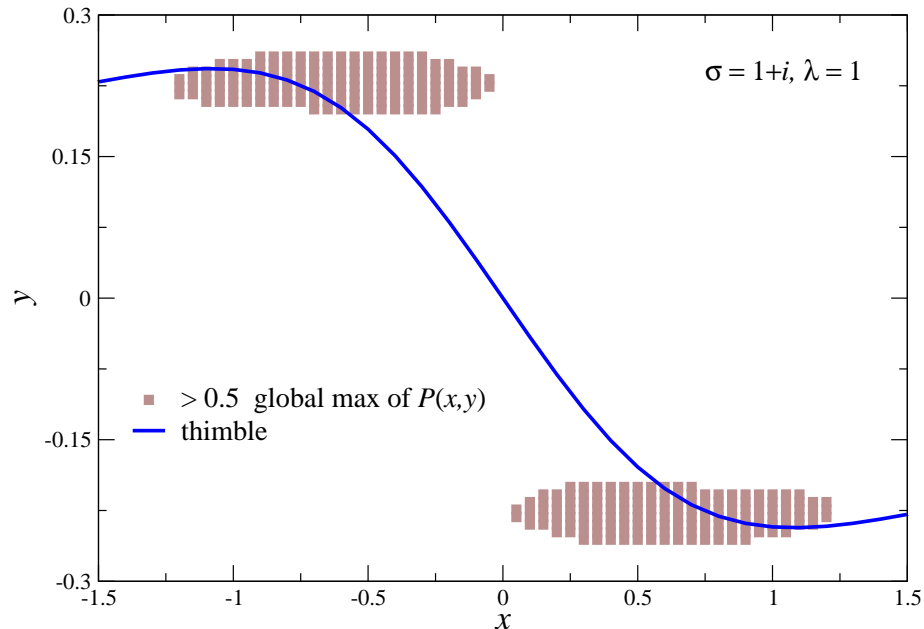
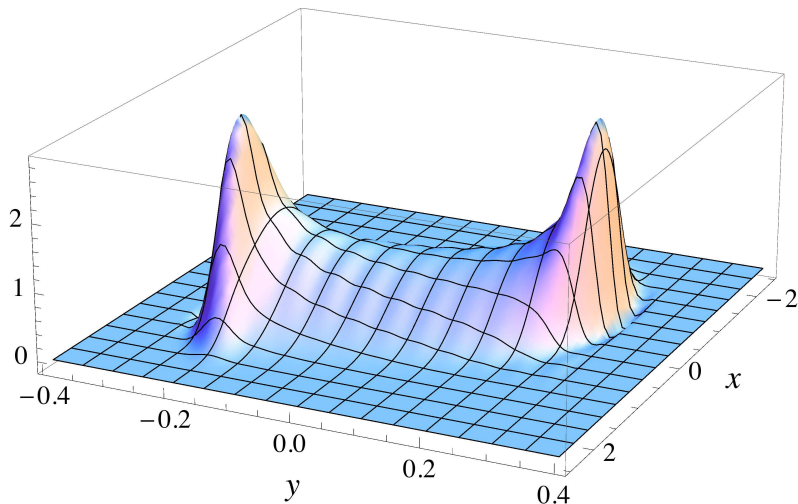
compare thimble and FP distribution $P(x, y)$



● thimble and $P(x, y)$ follow each other

Quartic model: thimbles

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



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

intriguing result: complex Langevin process finds the thimble – is this generic?

Langevin versus Lefschetz

compare evolution equations in more detail

- complex Langevin (CL) dynamics

$$\dot{x} = -\text{Re } \partial_z S(z) + \eta \qquad \dot{y} = -\text{Im } \partial_z S(z)$$

- Lefschetz thimble dynamics, with $z(t \rightarrow \infty) = z_k$

$$\dot{x} = -\text{Re } \partial_z S(z) \qquad \dot{y} = +\text{Im } \partial_z S(z)$$

\Rightarrow change in sign for y drift

Langevin:

- stable and unstable fixed points
- unstable runaways as $y \rightarrow \pm\infty$

thimbles:

- saddle points
- stable thimbles coming from $y \rightarrow \pm\infty$

Langevin versus Lefschetz

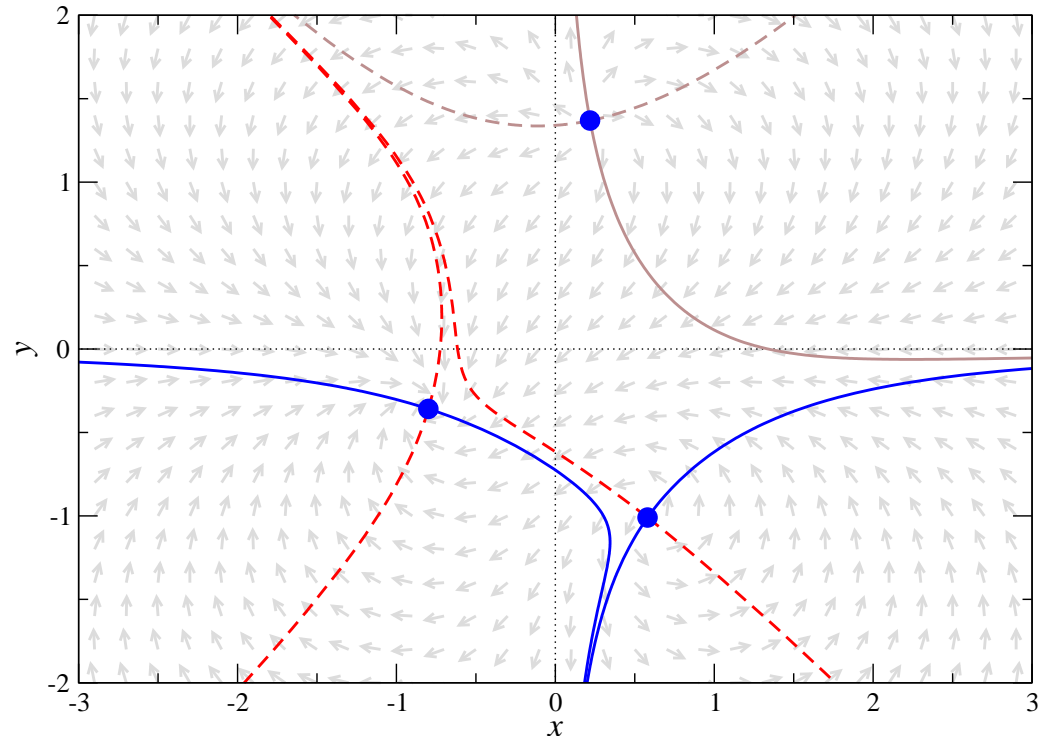
deform quartic model with linear term, break symmetry

$$S(z) = \frac{\sigma}{2}z^2 + \frac{1}{4}z^4 + hz$$

$$h \in \mathbb{C}$$

Langevin flow for

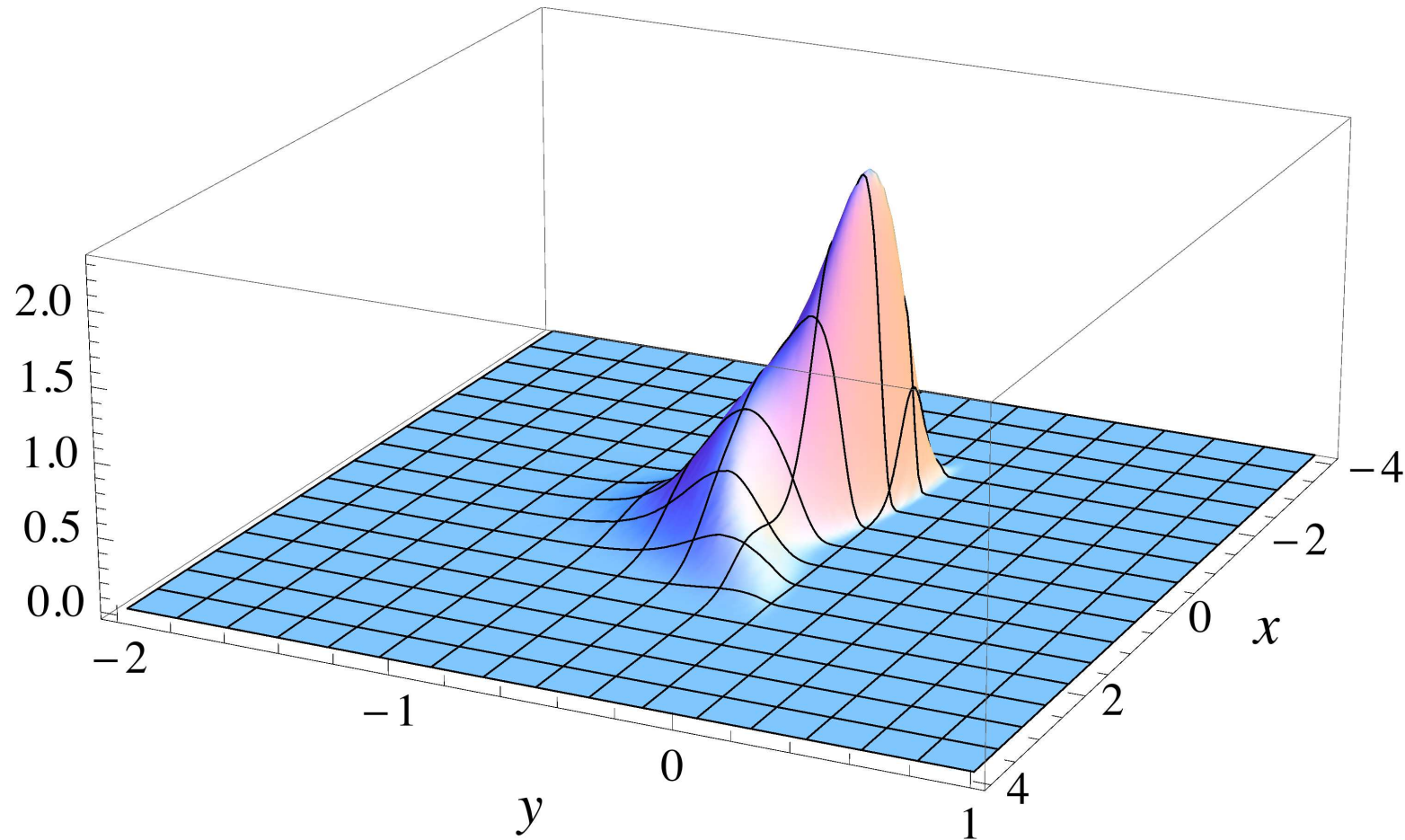
$$\sigma = 1, h = 1 + i$$



- one stable/two unstable fixed points for CL
- $y \rightarrow -\infty$ classical runaway trajectory
- two contributing thimbles (global phase problem) due to Stokes' phenomenon (1847)

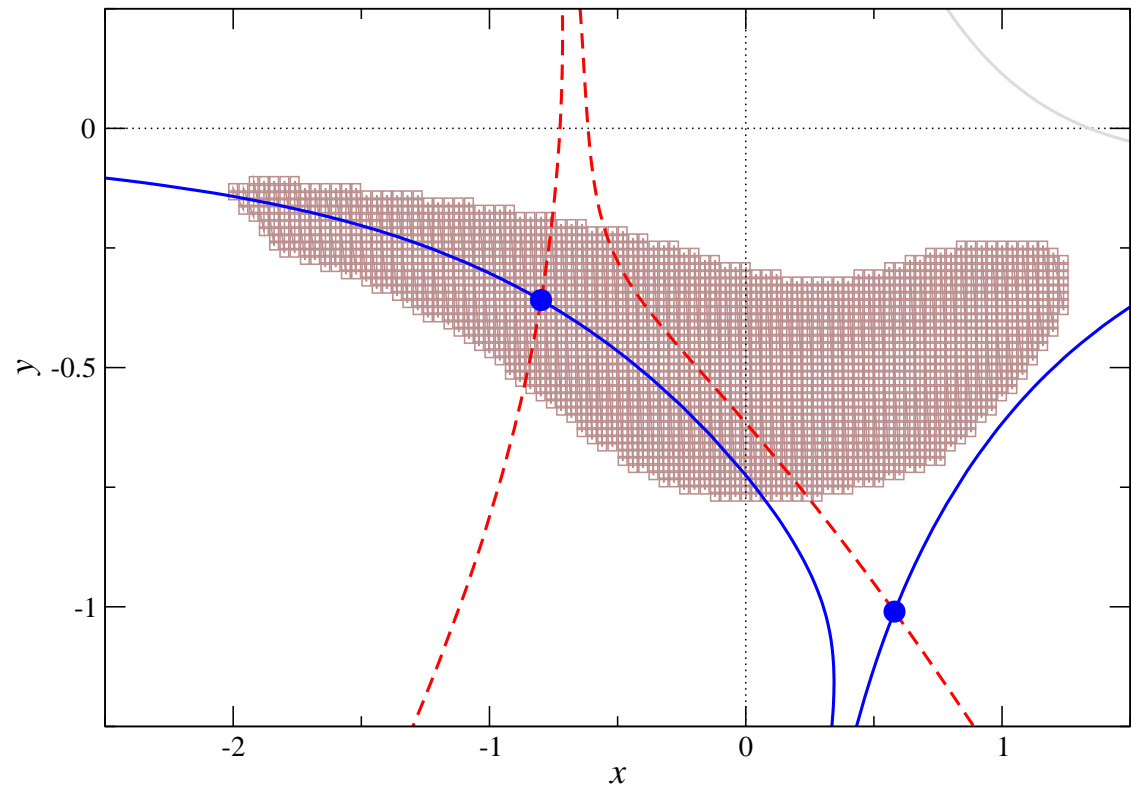
Langevin versus Lefschetz

histogram of $P(x, y)$ collected during CL simulation



Langevin versus Lefschetz

comparison of
Langevin distribution
with thimbles



- thimbles: both saddle points contribute
 - CL: unstable fixed point avoided
 - no role for second thimble in Langevin
- ⇒ distributions manifestly different

Other (more relevant) models

U(1) model with determinant

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

- presence of $\log \det$ of interest for CL and thimbles

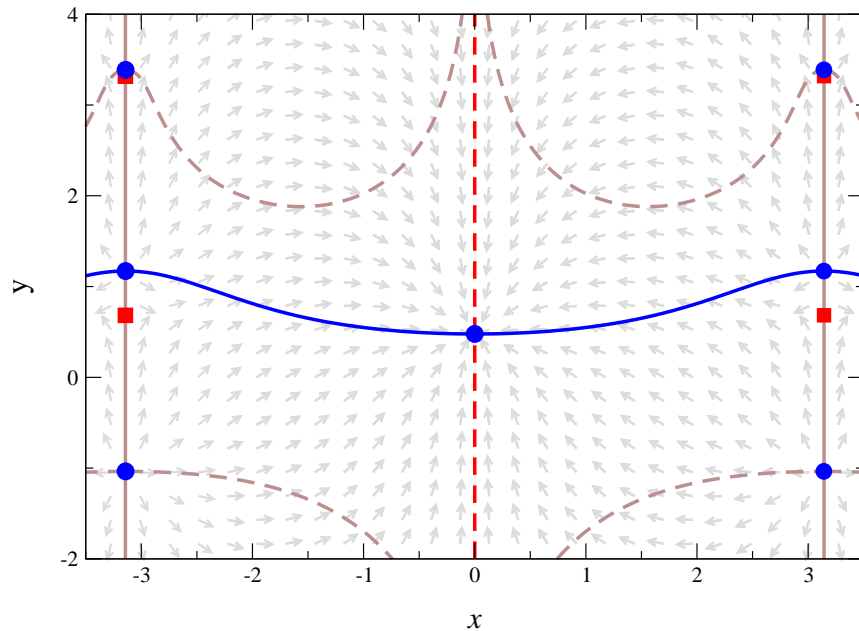
GA & Stamatescu 08, Mollgaard & Splittorff 13, Greensite 14

SU(2) one-link model with complex β

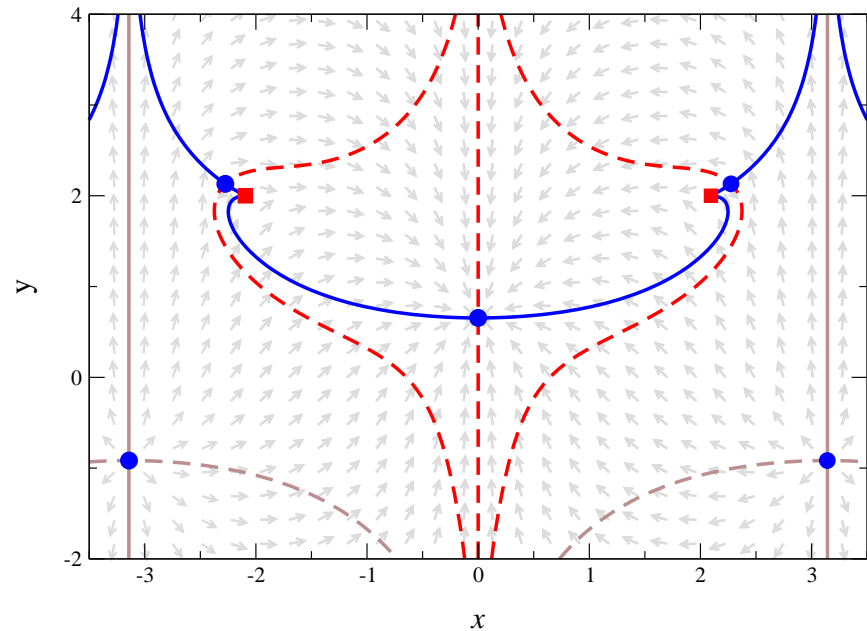
$$Z = \int dU e^{-S(U)} \quad S(U) = -\frac{\beta}{2} \text{Tr } U$$

- solvable with CL in different ways (gauge fixing, gauge cooling, ...)

U(1) model with determinant



$$\kappa = 1/2 < 1$$

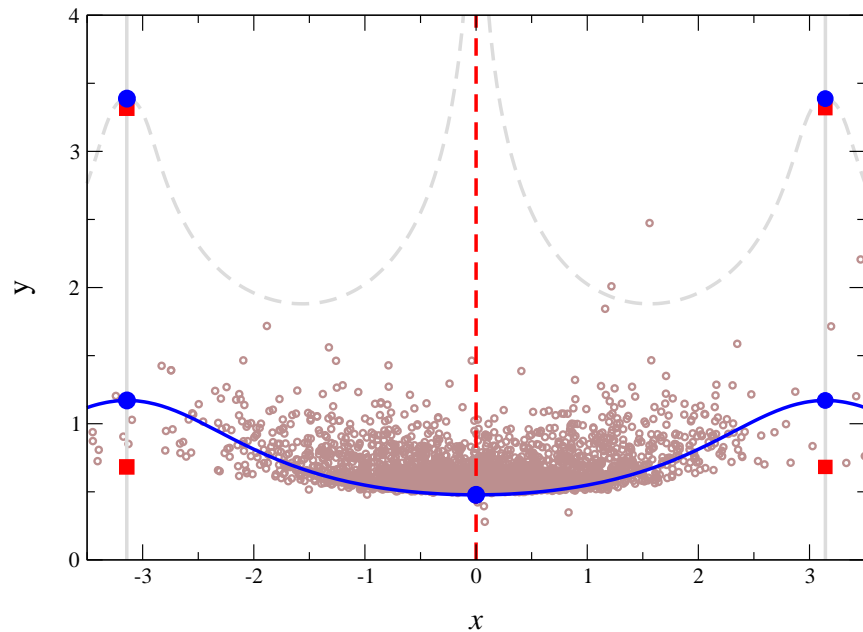


$$\kappa = 2 > 1$$

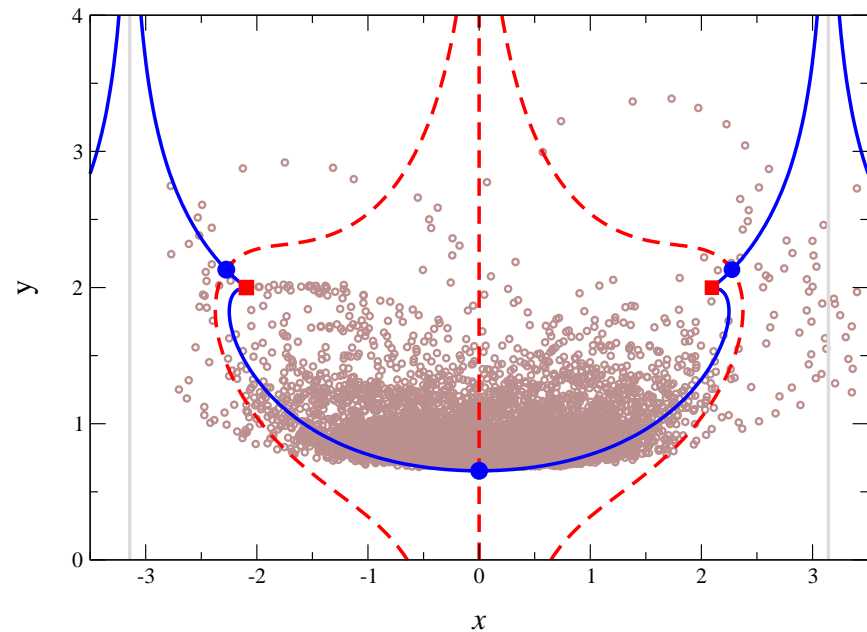
- arrows: Langevin drift
- blue dots: fixed points
- red squares: diverging drift, $\det = 0$

\Rightarrow new feature: thimbles can end, $\text{Im}S$ jumps

U(1) model with determinant



$$\kappa = 1/2 < 1$$



$$\kappa = 2 > 1$$

- dots: Langevin trajectory
- blue lines: contributing stable thimbles

Langevin distribution follows thimbles
spread in y direction when $\kappa > 1$

SU(2) model

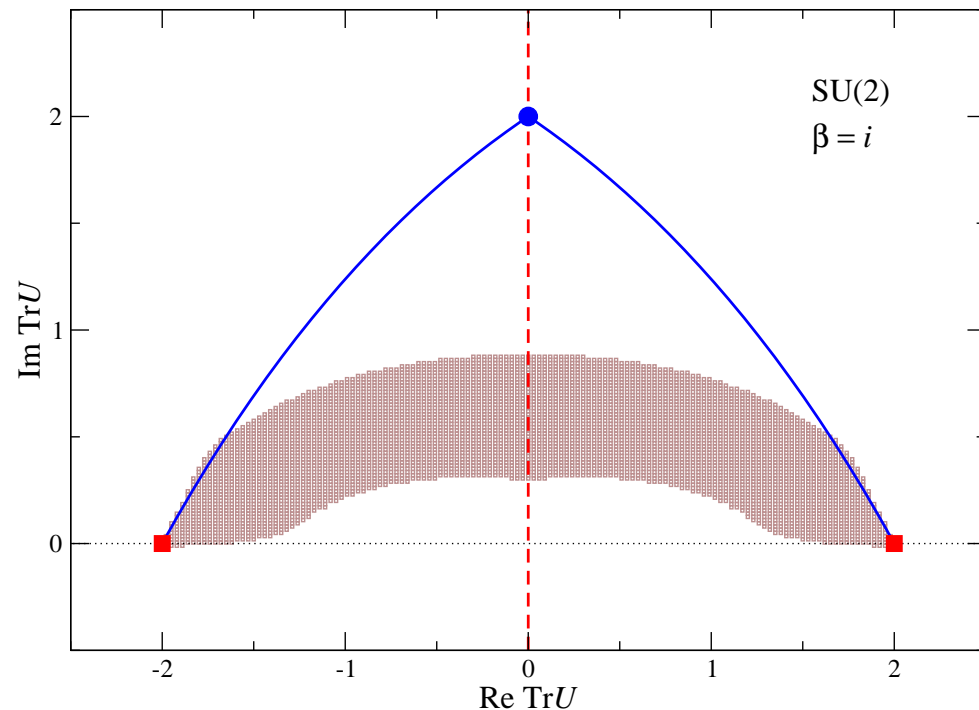
special case $\beta = i$

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
 $\frac{1}{2} \text{Tr } U = \cos z$
 $= u + iv$
- CL distribution
pinched by thimbles



Summary

exploring the complex plane: thimbles and Langevin

- location of distributions related but not identical
- weight distributions typically different
- repulsive fixed points in Langevin dynamics avoided

thimbles in simple models:

- *all* contributing thimbles should be included
- residual sign problem is relevant

in field theory both seem less stringent, why?