Some comments on holomorphic flow, thimbles and the sign problem

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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

$\Rightarrow$ QCD phase diagram has not yet been determined non-perturbatively

Outline

- complex actions and holomorphicity
- Lefshetz thimbles
- holomorphic flow
- open questions
- summary

mostly preliminary (hand-drawn figures...)

QCD partition function on the lattice

$$Z = \int DU\, D\bar{\psi} D\psi\, e^{-S} = \int DU\, e^{-S_{\rm YM}} \det M$$

with

$$S = S_{\rm YM} + \bar{\psi} M \psi$$

- (very) high-dimensional integral
- importance sampling if integrand is real and positive
- at nonzero baryon chemical potential, $\det M \in \mathbb{C}$

sign problem

- consider integrals with complex integrands

Complex actions and holomorphicity

simple integrals

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

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

are done in Kindergarten by deforming integration contour

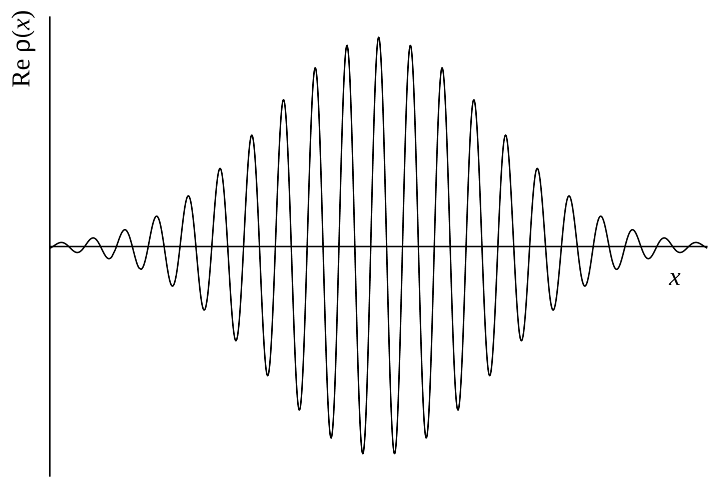
- stationary phase/saddle point expansion
- complex contour integral
- . . .

Complex actions and holomorphicity

in view of the sign problem:

replace oscillating integrals with well-behaved ones

- dominant configurations in the (path) integral?



- a real and positive distribution in the complex plane?

Complex actions

various approaches relying on holomorphicity:

go into the complex plane

- complex Langevin dynamics/stochastic quantisation

  GA, Seiler, Sexty, Stamatescu, Jäger, Attanasio ..., 08–

- saddle point/steepest descent: Lefschetz thimbles

  Witten 10, di Renzo et al, 12–, ...

- (anti)-holomorphic flow

  Alexandru, Bedaque et al, 16–

Deforming the integration contour

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

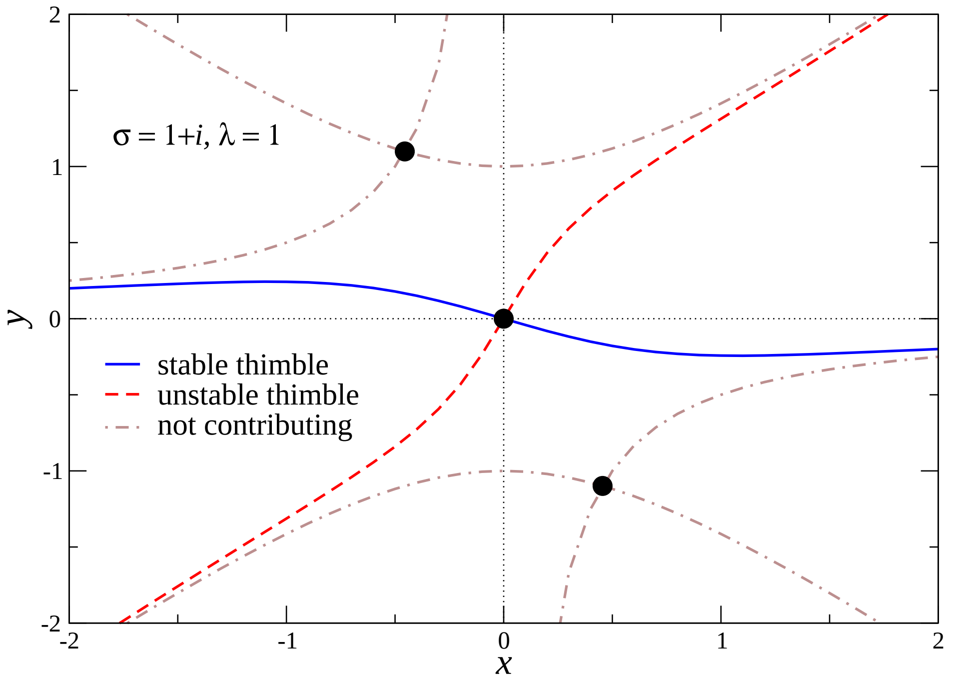
complex mass parameter $\sigma = A + iB$, $\lambda \in \mathbb{R}$

often used toy model Ambjorn & Yang 85, Klauder & Petersen 85, Okamoto et al 89, Duncan & Niedermaier 12, GA et al 14

deform the contour (blue line)

sign problem strongly diminished

how to determine deformation(s)?



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 $\mathcal{K}_k$
- $\mathrm{Im}\, S(z)$ constant along thimble k

integrate over stable thimbles, with proper weighting

Lefschetz thimbles

- stable thimble equation $\mathcal{J}_k$

$$\dot{z} = -\overline{\partial_z S(z)}$$

with $z(t \to \infty) = z_k$

$$\mathrm{Im} S(z_{\mathrm{thimble}}) = \mathrm{Im} S(z_k) = \text{cst}$$

- unstable thimble equation $\mathcal{K}_k$

$$\dot{z} = -\overline{\partial_z S(z)}$$

with $z(t \to -\infty) = z_k$ or $t \to -t$

Lefschetz thimbles

generalised saddle point integration/steepest descent:

- integrate over stable thimbles

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

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

- 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 $e^{-i\mathrm{Im}S(z_k)}$

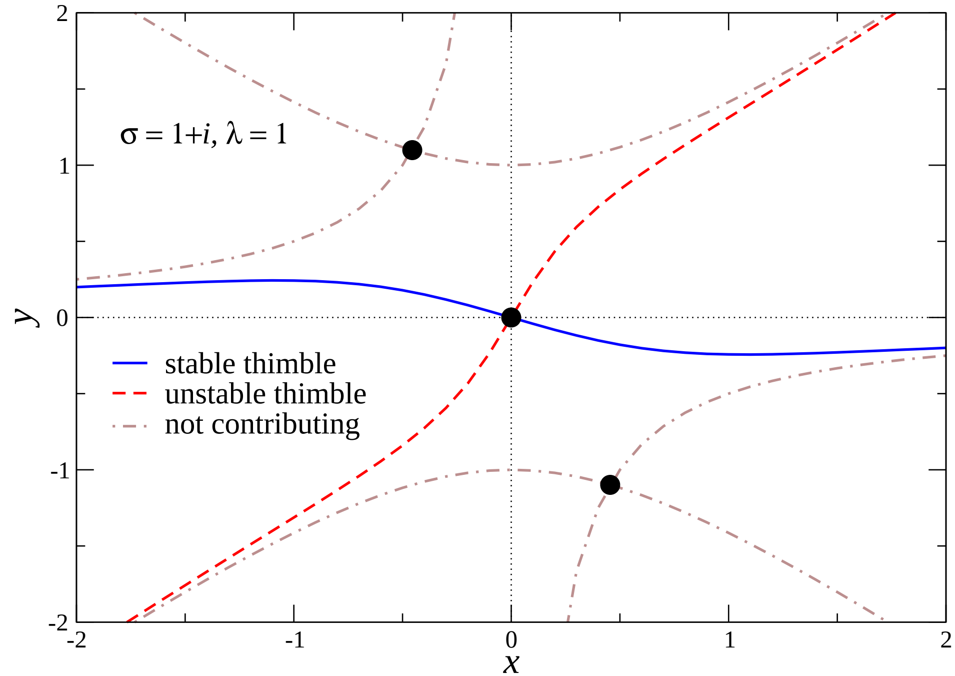
Lefschetz thimbles for quartic model

- 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

Thimbles: issues

some hurdles:

all thimbles should be included in principle

- how to determine them
- global sign problem

for each thimble

- residual sign problem due to complex jacobian
- computation of determinant numerically very expensive

but some success has been achieved

Recent development: holomorphic flow

attempts to alleviate hurdles:

- no need to determine thimbles precisely
- due to holomorphicity, any deformation is fine
- determine "optimal" contour algorithmically

(anti)-holomorphic flow Alexandru, Bedaque et al, 16-

other related approaches:

- sign-optimised manifolds Alexandru, Bedaque, Lamm, Lawrence 18
- path optimisation Mori, Kashiwa & Ohnishi 17, Bursa & Kroyter 18

Holomorphic flow

main idea:

- any contour is fine
- avoid singularities
- preserve analytically

potential issues:

- ergodicity
- complex jacobian due to deformation
- residual sign problem
- expensive

Holomorphic flow

thimble equation: $\dot{z} = -\overline{\partial_z S}$

flow equation: $\dot{z} = +\overline{\partial_z S}$

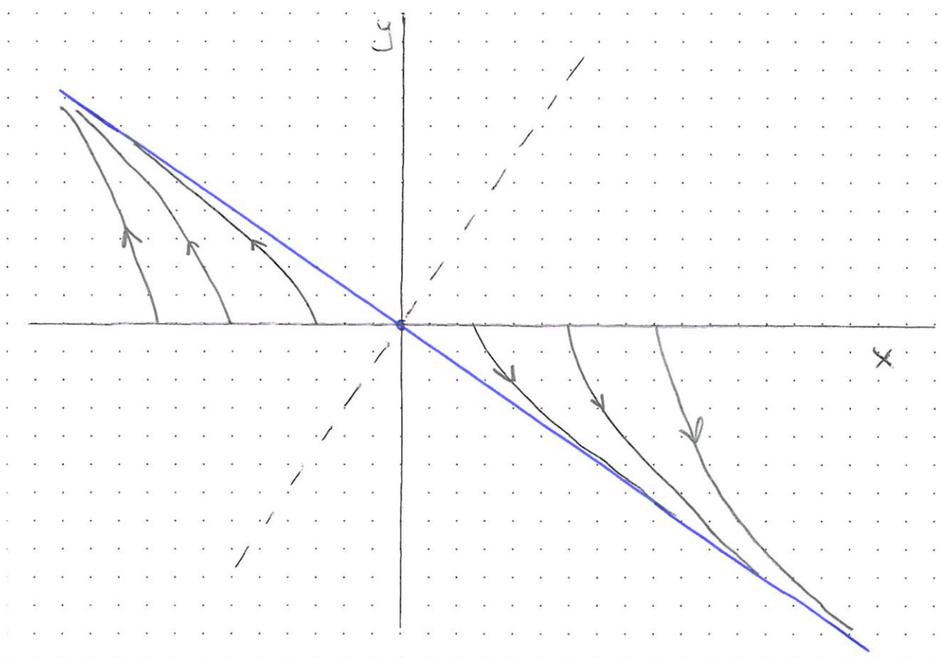
comparison with thimble dynamics

because of change of sign/direction of flow time:

- as $t \to \infty$
  flow moves towards thimble at $z \to \pm\infty$
  not $z \to z_k$

Example 1: Gaussian flow

- simple Gaussian model: $S = \frac{1}{2}\sigma z^2$ $\qquad \sigma = A + iB$
- flow and thimbles solved analytically
- trivial jacobian



- exponential flow towards thimble at $z \to \pm\infty$

Holomorphic flow

thimble equation: $\dot{z} = -\overline{\partial_z S}$

flow equation: $\dot{z} = +\overline{\partial_z S}$

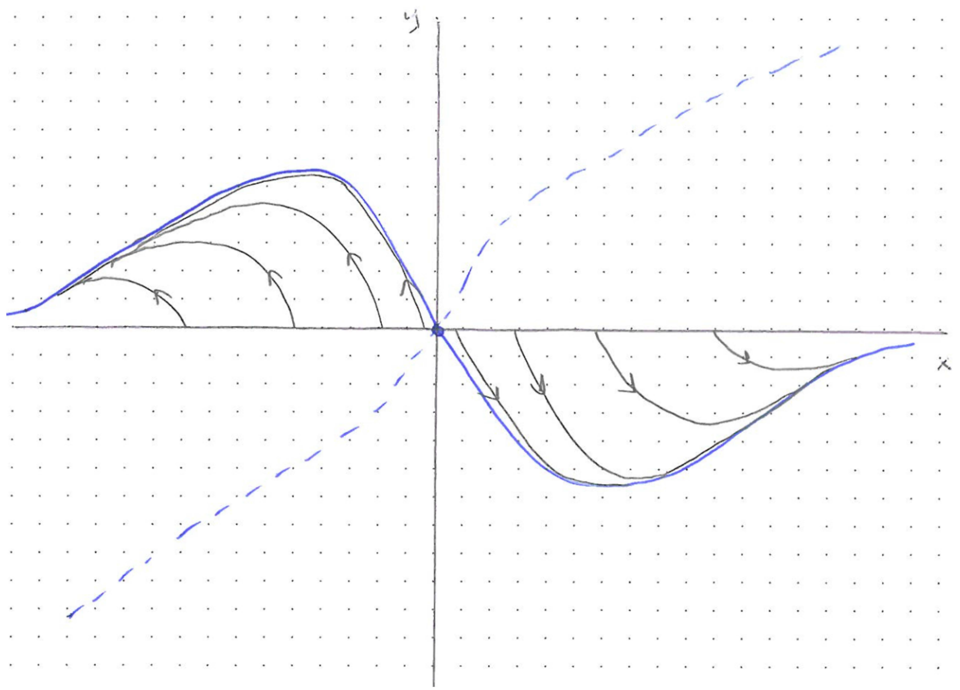
how does the weight/action change under flow?

$$\frac{dS}{dt} = \frac{\partial S}{\partial z}\frac{\partial z}{\partial t} = |\partial_z S|^2 \geq 0$$

- $\mathrm{Im}S(z)$ does not evolve in flow time
- $\mathrm{Re}S(z)$ increases during flow
- region around $z = z_k$ becomes more important
- sample region closer to z_k, $\mathrm{Im}S(z)$ approximately cst

Example 2: with interaction

- simple model: $S = \frac{1}{2}(A + iB)z^2 + \frac{\lambda}{4}z^4 \qquad A > 0$
- flow and thimbles solved analytically
- nontrivial jacobian



- exponential flow towards thimble at $z \to \pm\infty$

Holomorphic flow

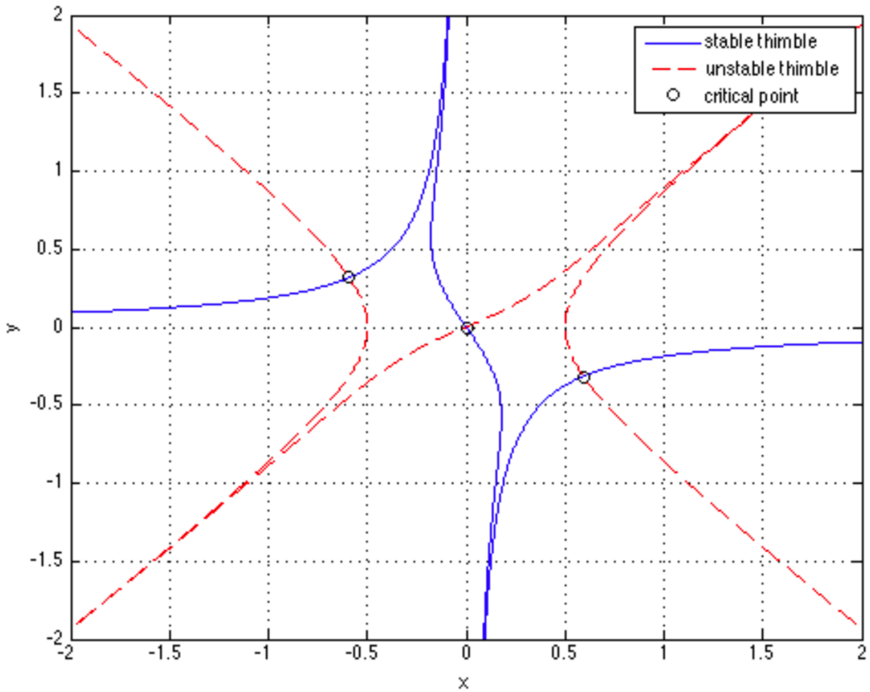
in both cases:

- $\mathrm{Im} S = \frac{1}{2} B z^2$ is preserved under flow
- only region exponentially close to $z = 0$ contributes
- sign problem alleviated since $\mathrm{Im} S = \frac{1}{2} B z^2 \to 0$

what about more than one contributing thimble?

Example 3: with interaction

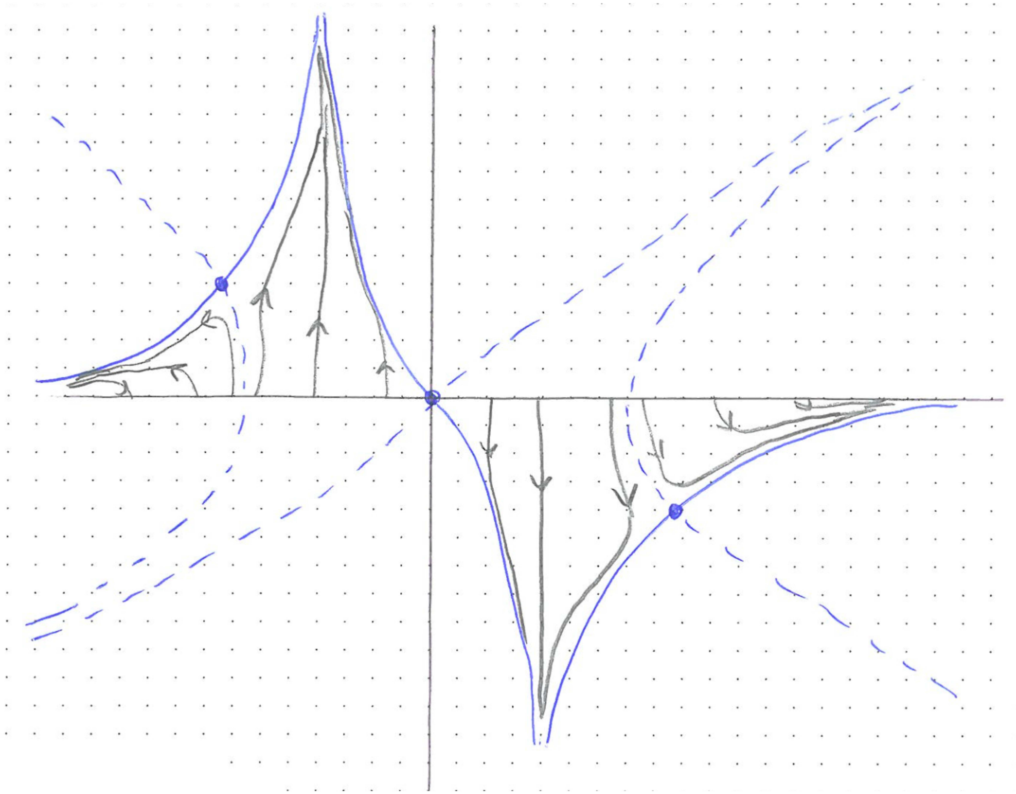
- simple model: $S = \frac{1}{2}(A + iB)z^2 + \frac{\lambda}{4}z^4 \qquad A < 0$
- all critical points contribute: 3 thimbles



di Renzo & Eruzzi 15

Example 3: with interaction

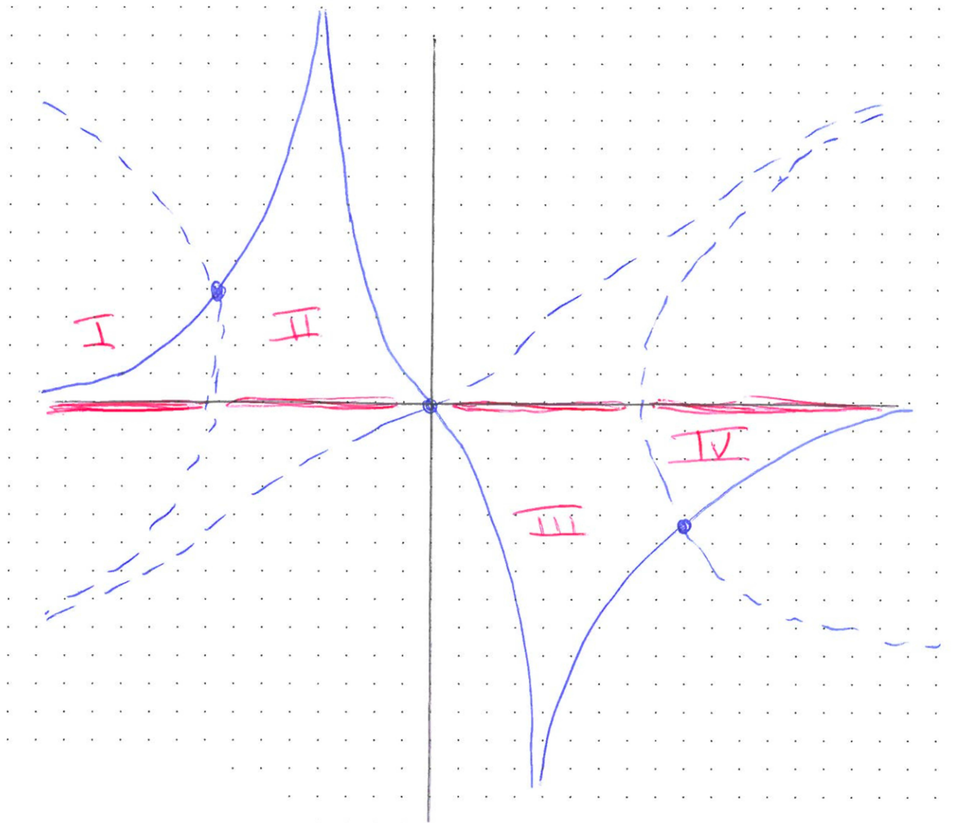
- simple model: $S = \frac{1}{2}(A + iB)z^2 + \frac{\lambda}{4}z^4 \qquad A < 0$
- unstable thimbles are separatrices
- disjoint regions



- under flow, trajectories trapped close to thimbles

Example 3: with interaction

- unstable thimbles are separatrices: disjoint regions
- potential problems with ergodicity
- flow does not allow for tunnelling between regions

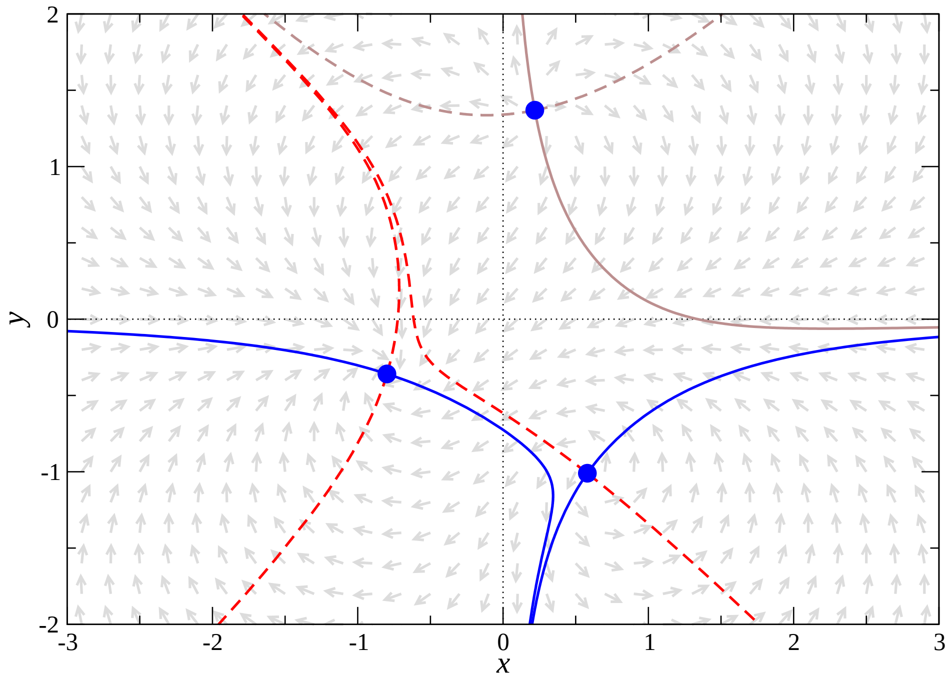


- chose weight for each region correctly

Example 4: less symmetry

$$S = \frac{1}{2}\sigma z^2 + \frac{\lambda}{4} z^4 + hz \qquad\qquad h \in \mathbb{C}$$

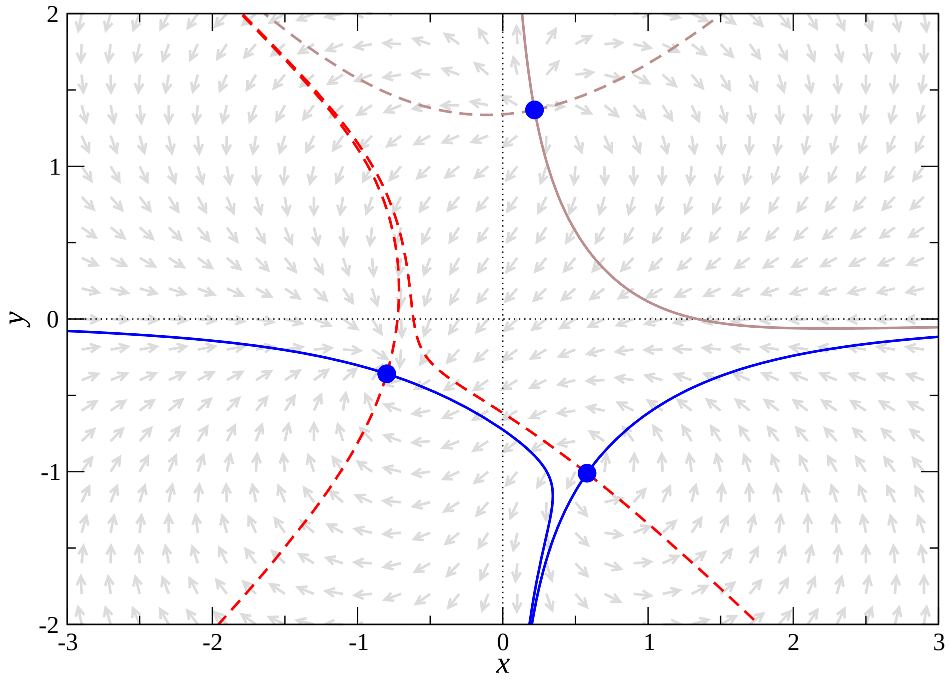
- critical points not related by symmetry
- two thimbles contribute, one more dominant
- one thimble does not contribute



GA, Bongiovanni, Seiler & Sexty 15

Example 4: less symmetry

- unstable *and* stable thimbles can be separatrices
- small regions on real axis can dominate final answer
- one stable thimble does not contribute but separates complex plane



Lessons

one dimensional integrals

- disjoint configuration space
- sampling of initial conditions on real axis should reflect contribution to final answer
- jump between regions respecting detailed balance (?)

higher dimensional models/field theory

- $\mathbb{R}^N \to \mathbb{R}^{2N}$
- thimbles are N dimensional
- no longer separatrices
- but flow attracted to thimbles: danger of trapping
- noncontributing thimbles can pose barrier

Summary

deforming the path integral

- Lefschetz thimbles and holomorphic flow
- barriers and disjoint regions

in high-dimensional theories

- trapped regions?
- ergodicity?
- faithful sampling of initial conditions for flow?