Simulating low dimensional QCD on Lefschetz thimbles

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Thimble

A thimble is a bell or ring shaped sheath of a hard substance, such as bone, leather, metal or wood, which is worn on the tip or middle of a finger or the thumb to help push a needle while sewing and to protect the finger/thumb from being pricked.

[source: Textile Research Centre (TRC), Leiden, The Netherlands]

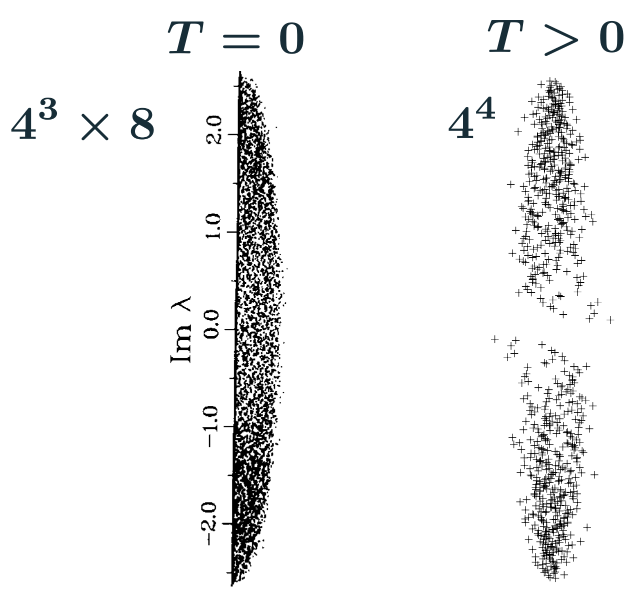
Motivation: The QCD sign problem

The QCD partition function

$$Z(T,V,m,\mu) = \int \mathcal{D}U \underbrace{\det M[U]}_{\text{complex for } \mu > 0} e^{-S_G[U]}$$

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

Lattice Dirac spectrum



Barbour *et al.*, 1986 Muroya *et al.*, 2003

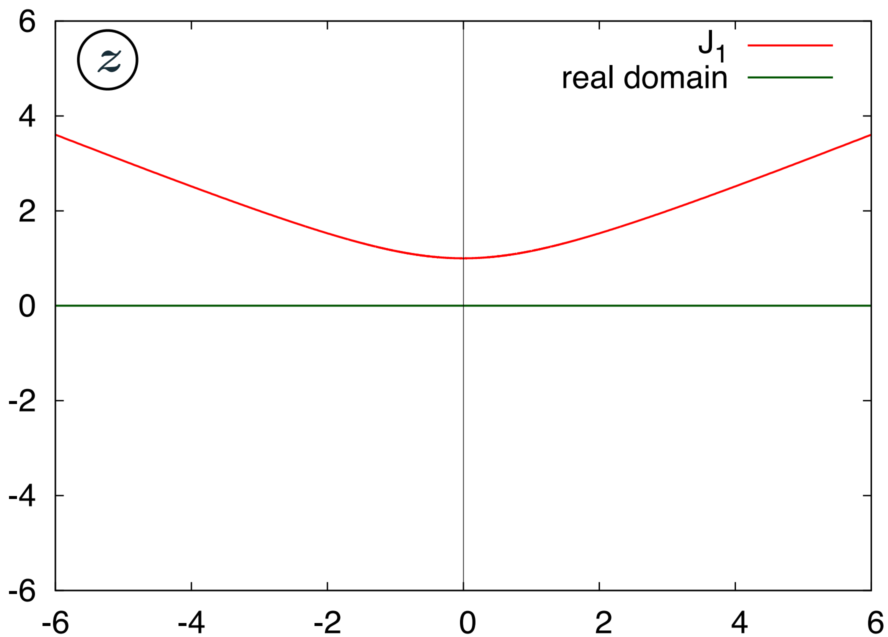
- standard MC techniques not applicable
- highly oscillatory integral with exponentially large cancellations

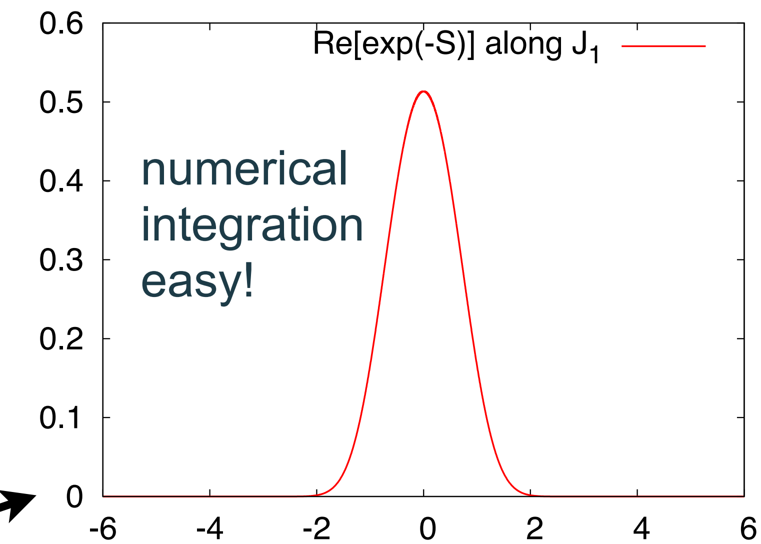
Idea:
Deforming the domain of integration

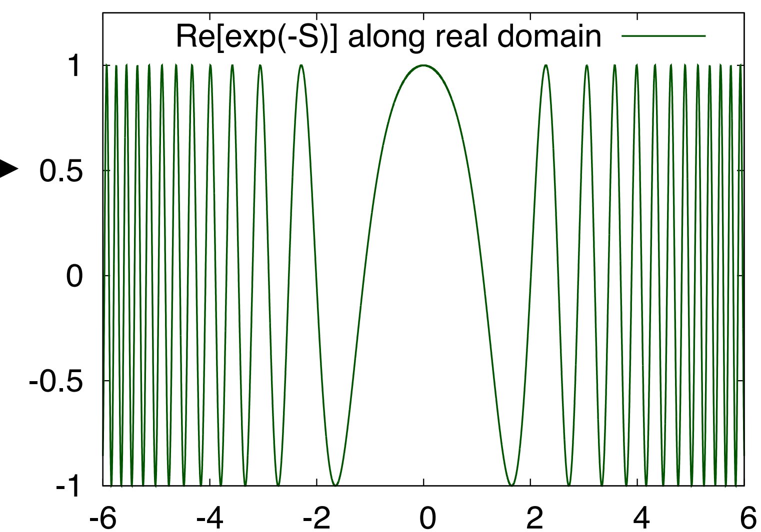
Standard 1d-example: the Airy integral

$$\mathbf{Ai}[1] = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}x \;\; \exp\left\{ i \left(\frac{x^3}{3} + x \right) \right\}$$

$$x \rightarrow z = x + iy$$







numerical integration hopeless!

see also Witten: 1001.2933, 1009.6032

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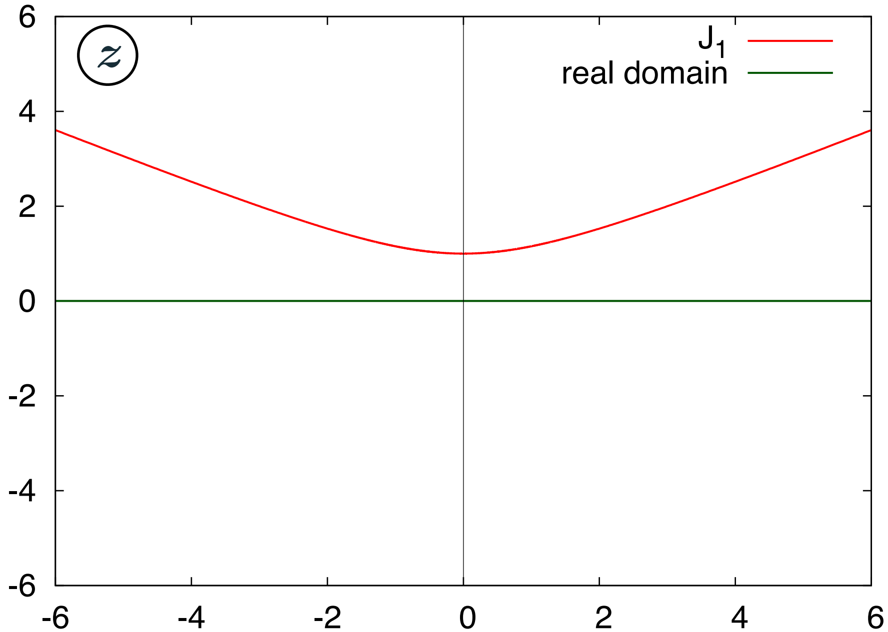

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Theory behind: Picard-Lefschetz theory

- use the real valued function $S_R(z) = \mathrm{Re}[-i(z^3/3 + z)]$ as a Morse function

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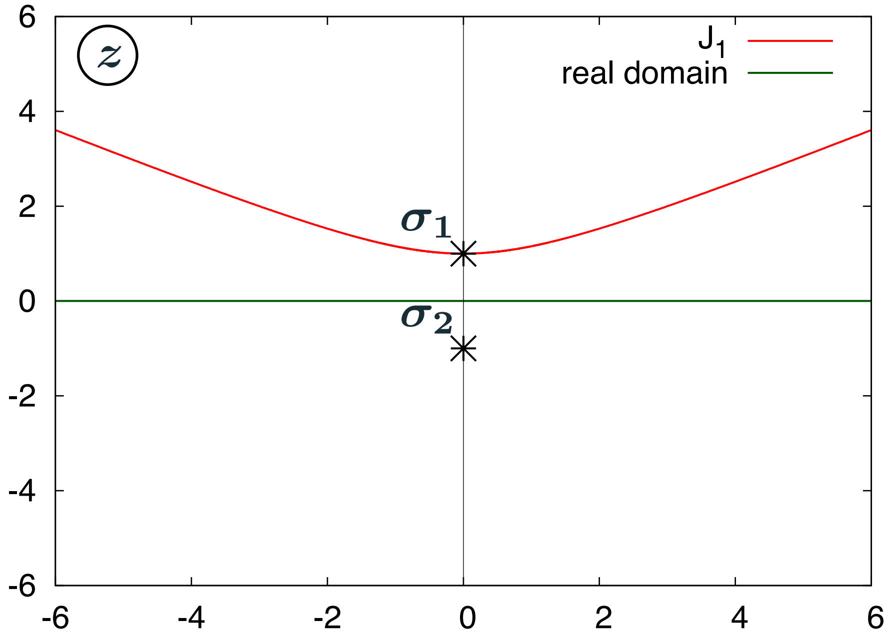

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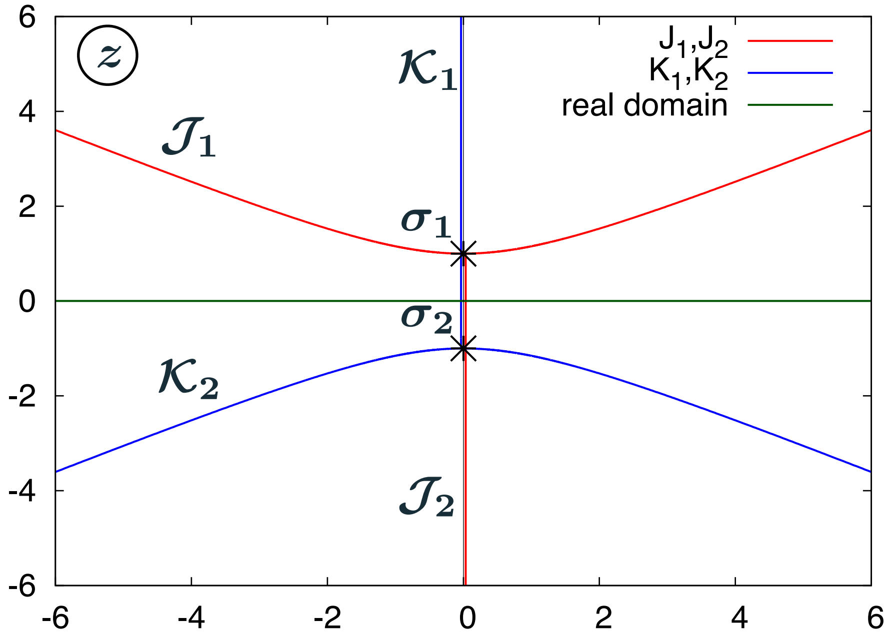

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- find all separated saddle points (σ_i)
- associated with each saddle point (σ_i), find one stable ($\mathcal{J}_i$) and one unstable thimble ($\mathcal{K}_i$) as solutions of the steepest descent/ascent flow equation

$$\frac{\mathrm{d}z}{\mathrm{d}t} = \mp\nabla S_R(z)$$

(note: $S_I(z)$ remains const. along flow)

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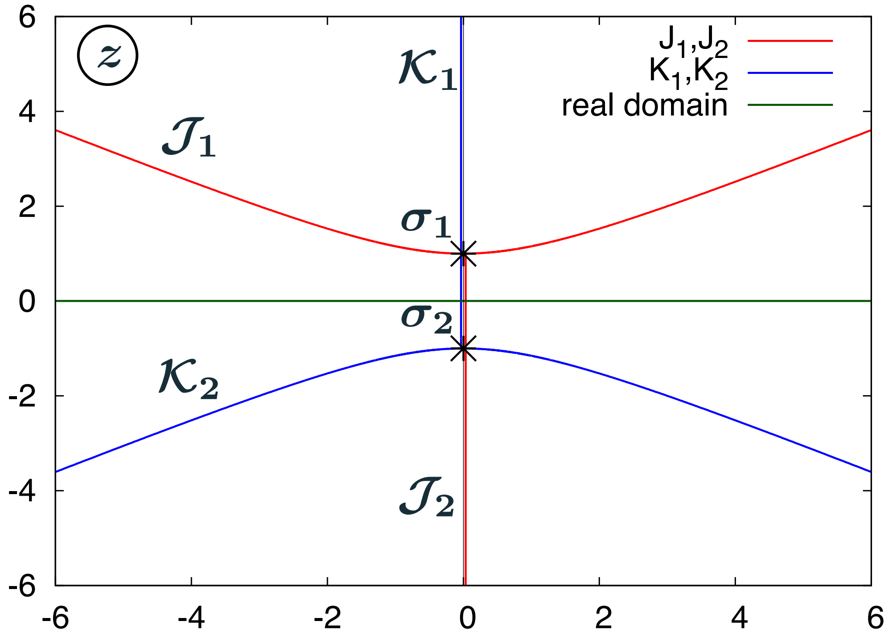

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- decompose original integral into thimbles

$$\int_{\mathbb{R}} \mathrm{d}z\; e^{-S(z)} = \sum_i n_i\; e^{-S_I(\sigma_i)} \int_{J_i} \mathrm{d}z\; e^{-S_R(z)}$$

(here: $n_1 = 1,\; n_2 = 0,\; S_I(\sigma_1) = 0$)

Idea:
Deforming the domain of integration

Original domain of integration

U^{4V} $\qquad U_{x,\nu} \in \mathrm{SU}(3)$ $\qquad$ real dim. $4 \times V \times 8$

$$U = \exp\left\{-i \sum_a \omega_a T_a\right\}$$

Complexified space

$\tilde{U}^{4V}$ $\qquad \tilde{U}_{x,\nu} \in \mathrm{SL}(3,\mathbb{C})$ $\qquad$ real dim. $4 \times V \times 8 \times 2$

New domain(s) of integration: Lefschetz thimble

$\mathcal{J}_0 + \mathcal{J}_1 + \cdots$ $\qquad$ real dim. $4 \times V \times 8$

$\mathcal{J}_0 := \Big\{ \tilde{U}_{x,\nu} \mid U(\tau)$ is solution of the SD equation with $U(0) = \tilde{U}_{x,\nu}$ and $U(\tau \to \infty) = \mathcal{N} \Big\}$

here $\mathcal{N}$ denotes the gauge orbit of the unity configuration

Open questions:

How many relevant thimbles are there in full QCD?

How to sample them?

- Langevin on the thimble (Aurora-algorithm)
  Cristoforetti et al., PRD 86 (2012) 074506
- HMC on the thimble
  Fujii et al., JHEP 1310 (2013) 147
- Use a map of the thimble (projection-, contraction-algorithm)
  A. Mukherjee et al., PRD 88 (2013) 051502; A. Alexandru et. al., PRD 93 (2016) 014504
- Sample SD paths on the thimble
  Di Renzo et al., PRD 88 (2013) 051502

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How to sample them?

How to combine results from different thimbles?

- input a number of physical quantities to determine relative weights

Di Renzo et al., PRD 88 (2013) 051502

$$X_i = \frac{\left\langle e^{i\phi} O_i \right\rangle_0 + \alpha_1 \left\langle e^{i\phi} O_i \right\rangle_1 + \alpha_2 \left\langle e^{i\phi} O_i \right\rangle_2}{\left\langle e^{i\phi} \right\rangle_0 + \alpha_1 \left\langle e^{i\phi} \right\rangle_1 + \alpha_2 \left\langle e^{i\phi} \right\rangle_2} \quad , \quad i = 1, 2 \quad , \quad \alpha_i = \frac{n_i e^{S_I(\sigma_i)} Z_i}{n_0 e^{S_I(\sigma_0)} Z_0}$$

here ϕ denotes the residual phase (see **Cristoforetti et al., PRD 89 (2014) 114505**)

Open questions:

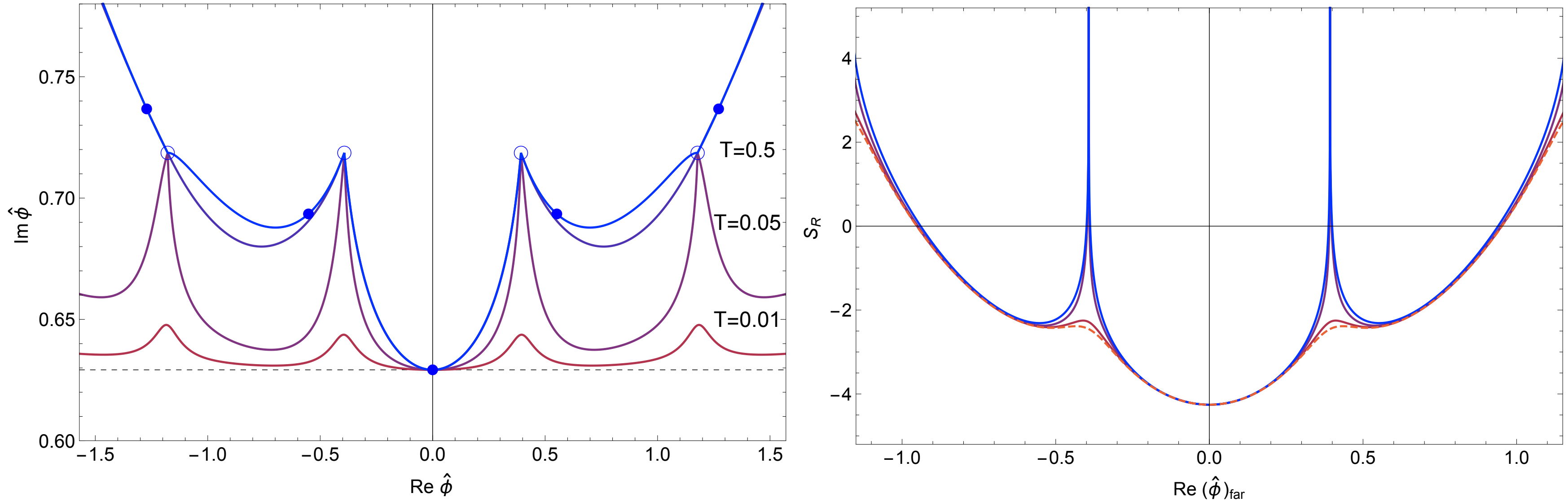
How many relevant thimbles are there in full QCD?

How to sample them?

How to combine results from different thimbles?

- input a number of physical quantities to determine relative weights
- sample multiple thimbles at once, or one manifold that comes arbitrary close to multiple thimbles

A. Alexandru et. al., JHEP 1605 (2016) 053



Open questions:

How many relevant thimbles are there in full QCD?

How to sample them?

How to combine results from different thimbles?

How to deal with the gauge orbits?

- perform simulations in a fixed gauge
- make use of the gauge gauge transformations

Systems studied so far:

ϕ^4-theory

Cristoforetti et al., PRD 88 (2013) 051501; Fujii et al., JHEP 1310 (2013) 147

Cristoforetti et al., PRD 89 (2014) 114505

Hubbard model, one-site Hubbard model

A. Mukherjee et al., PRD 88 (2013) 051502

(0+1)dim. Thirring model

Fujii et al., JHEP 1511 (2015) 078; Fujii et al., JHEP 1512 (2015) 125;

Chiral random matrix model

Di Renzo et al., PRD 88 (2013) 051502

⋮ (also applications to QM-systems in real time)

Agenda:

QCD in (0+1) dim. with std. staggered quarks

- simulations in Polyakov loop diagonal form
- simulations with a general Polyakov loop

QCD in (n+1) dim. with std. staggered quarks

- simulations at strong coupling
- simulations away from strong coupling

Agenda:

QCD in (0+1) dim. with std. staggered quarks

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this talk :-)

QCD in (n+1) dim. with std. staggered quark

- simulations at strong coupling
- simulations away from strong coupling

not yet :-(

(0+1) dimensional QCD

partition function in the reduced form

$$Z^{(N_f)} = \int \mathrm{d}P \, \det{}^{N_f} \underbrace{[A + e^{\mu/T} P + e^{-\mu/T} P^{-1}]}_{D}$$

$$A = 2\cosh(\hat{\mu}_c) \mathbb{1}_3$$

$$\hat{\mu}_c = \operatorname{arcsinh}(\hat{m})$$

Bilic et al. Phys. Lett. B212 (1988) 83

(see e.g. Ammon et al., arXiv:1607.05027)

diagonalize Polyakov loop

$$P = \operatorname{diag}(e^{i\theta_1}, e^{i\theta_2}, e^{-i(\theta_1+\theta_2)})$$

$$J(\theta_1, \theta_2) = \frac{8}{3\pi^2} \sin^2\left(\frac{\theta_1 - \theta_2}{2}\right) \sin^2\left(\frac{2\theta_1 + \theta_2}{2}\right) \sin^2\left(\frac{\theta_1 + 2\theta_2}{2}\right)$$

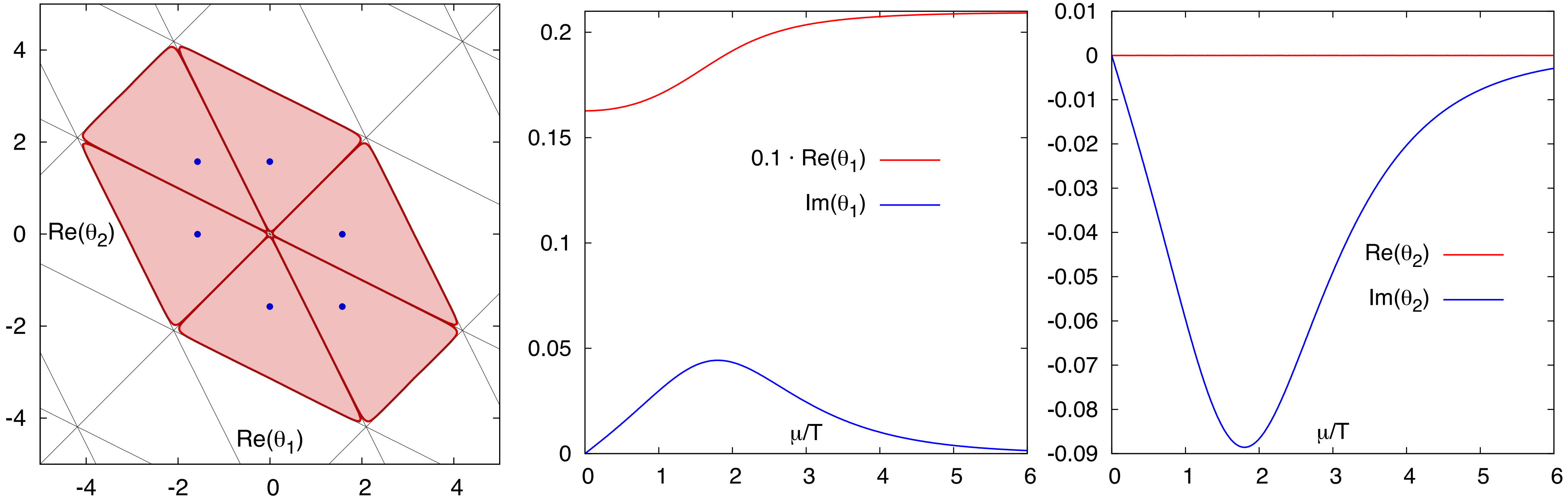
$$Z^{(N_f)} = \int \mathrm{d}\theta_1 \mathrm{d}\theta_2 \, e^{-S_{eff}(N_f, \theta_1, \theta_2)}$$

$$S_{eff} = -(\ln J + \operatorname{Tr} \ln D)$$

(0+1) dimensional QCD

find saddle points: minimize $||\nabla_z S^R_{eff}||$, **with** $z = (\mathrm{Re}\theta_1, \mathrm{Re}\theta_2, \mathrm{Im}\theta_1, \mathrm{Im}\theta_2)^t$

$\mu/T = 0 \qquad m/T = 0.2$



- thimbles are separated by lines of zero probability (infinite action)
- saddle points are μ-dependent
- all thimbles are equivalent (give the same contribution)

(0+1) dimensional QCD

find tangent space of the thimble at the saddle points:

diagonalize hessian $\partial_{z_i}\partial_{z_j}S^R_{eff}$ **(at the saddle point)**

- eigenvectors with positive eigenvalues span the tangent space

sample the thimble using the contraction algorithm (A. Alexandru et. al., PRD 93 (2016) 014504 **)**

$$< \mathcal{O} >= \int \mathrm{d}z \; \mathcal{O}(z) e^{-S_{eff}(z)} = \int \mathrm{d}\bar{z} \; \mathrm{det}J \; \mathcal{O}(z(\bar{z})) \; e^{-S_{eff}(z(\bar{z}))}$$

- $\bar{z}$ are elements of the tangent space
- $z(\bar{z})$ is defined by flowing $\bar{z}$ along the SA for a fixed time T (note: the SA flow is numerically stable)
- $J_{ij} = \partial z_i / \partial \bar{z}_j$ is the Jacobian, which is in practice obtained by transporting a parallelepipet $P(z)$ along the SA flow: $\mathrm{det}J = \mathrm{det}P(z(\bar{z}))/\mathrm{det}P(\bar{z})$
- $\mathrm{det}J$ has a complex phase (residual phase), sample according to $|\mathrm{det}J| e^{-S^R_{eff}}$ and take the residual phase into account by reweighting

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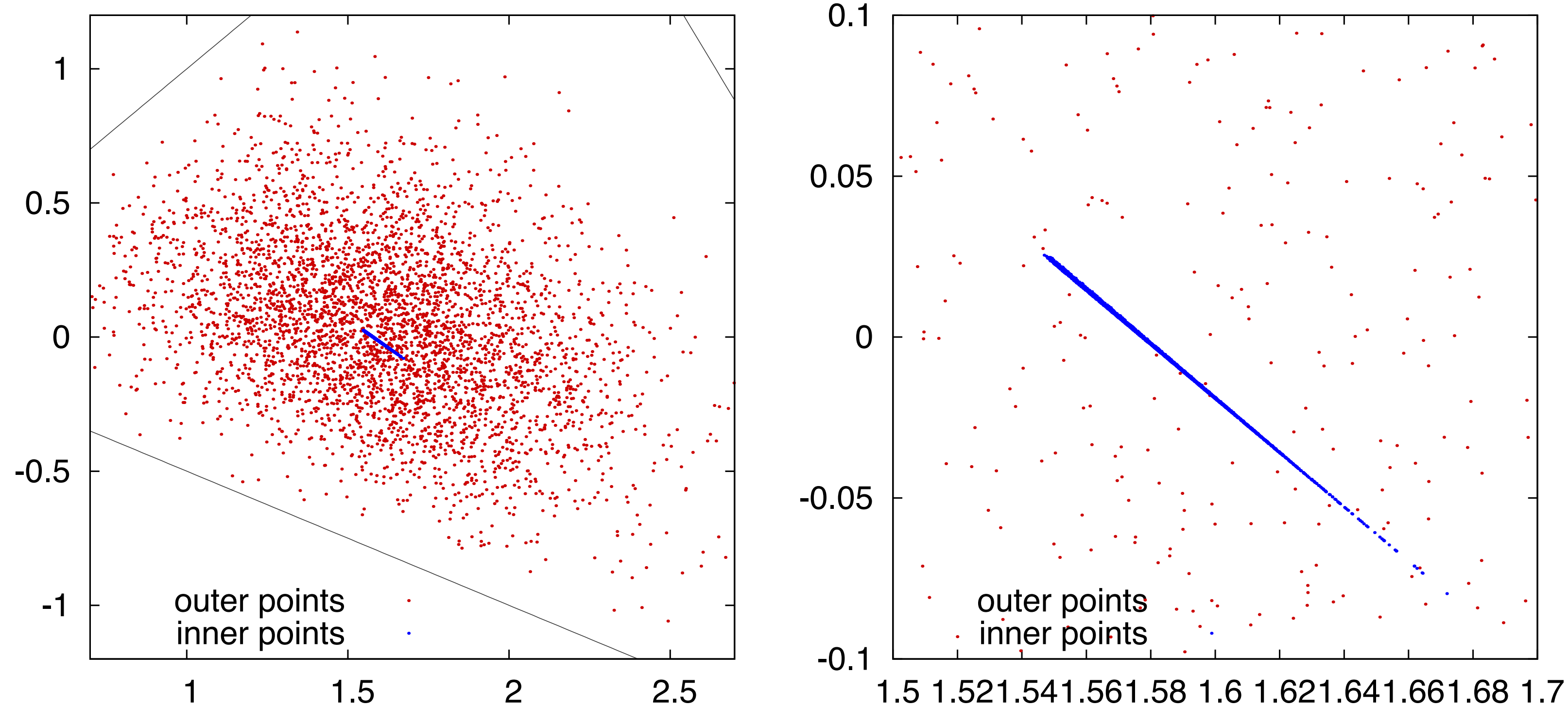
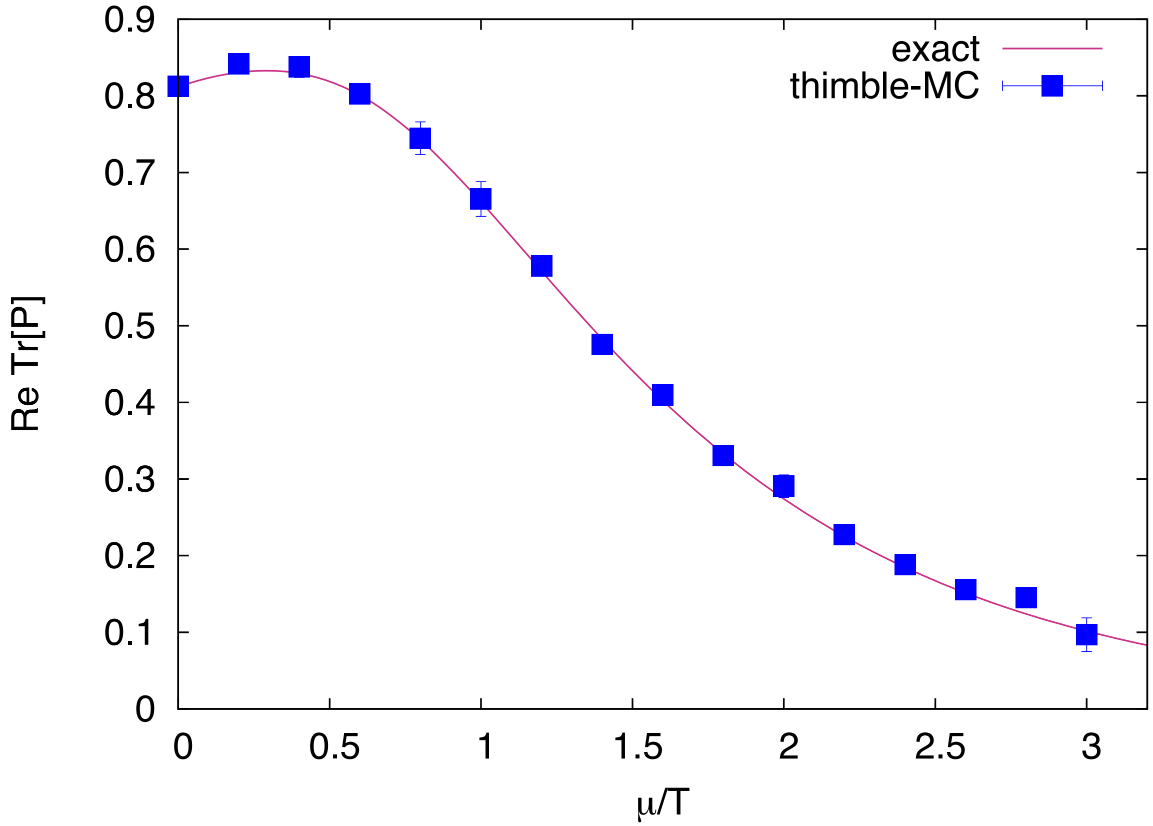


flow time:

$T = 0.7$

(0+1) dimensional QCD

results for the Polyakov loop:



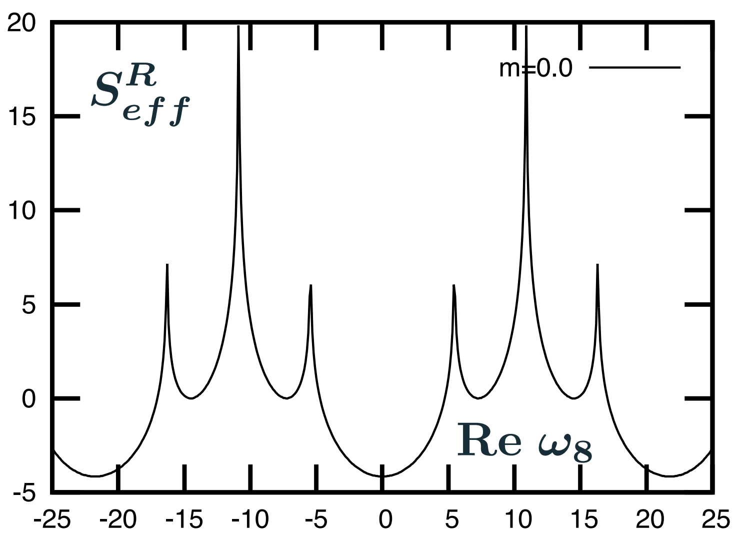
- exact results are reproduced
- only one relevant thimble found

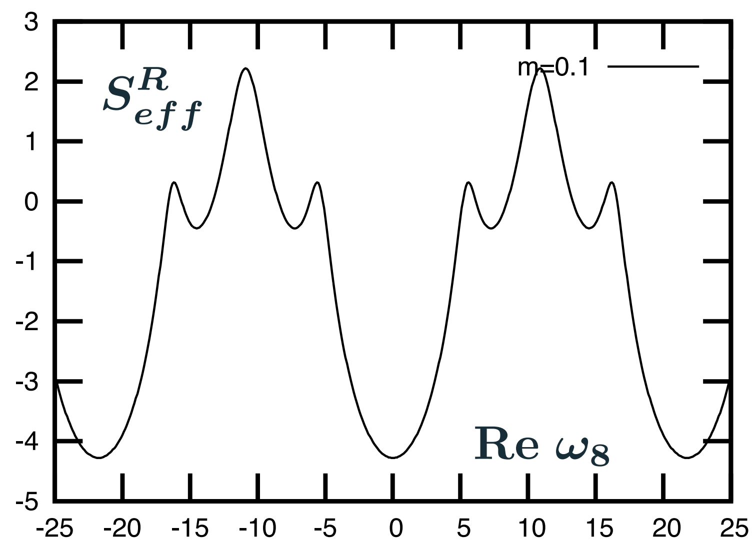
(0+1) dimensional QCD

sample non-diagonal Polyakov loops $P = \exp\left\{-i\sum_a \omega_a T_a\right\}$

fist step: find saddle points (now in 16 dim.)

$\mu/T = 0$





- find 3 thimbles, related to Z(3) symmetry
- at m=0, the thimbles are separated by singular points

(0+1) dimensional QCD

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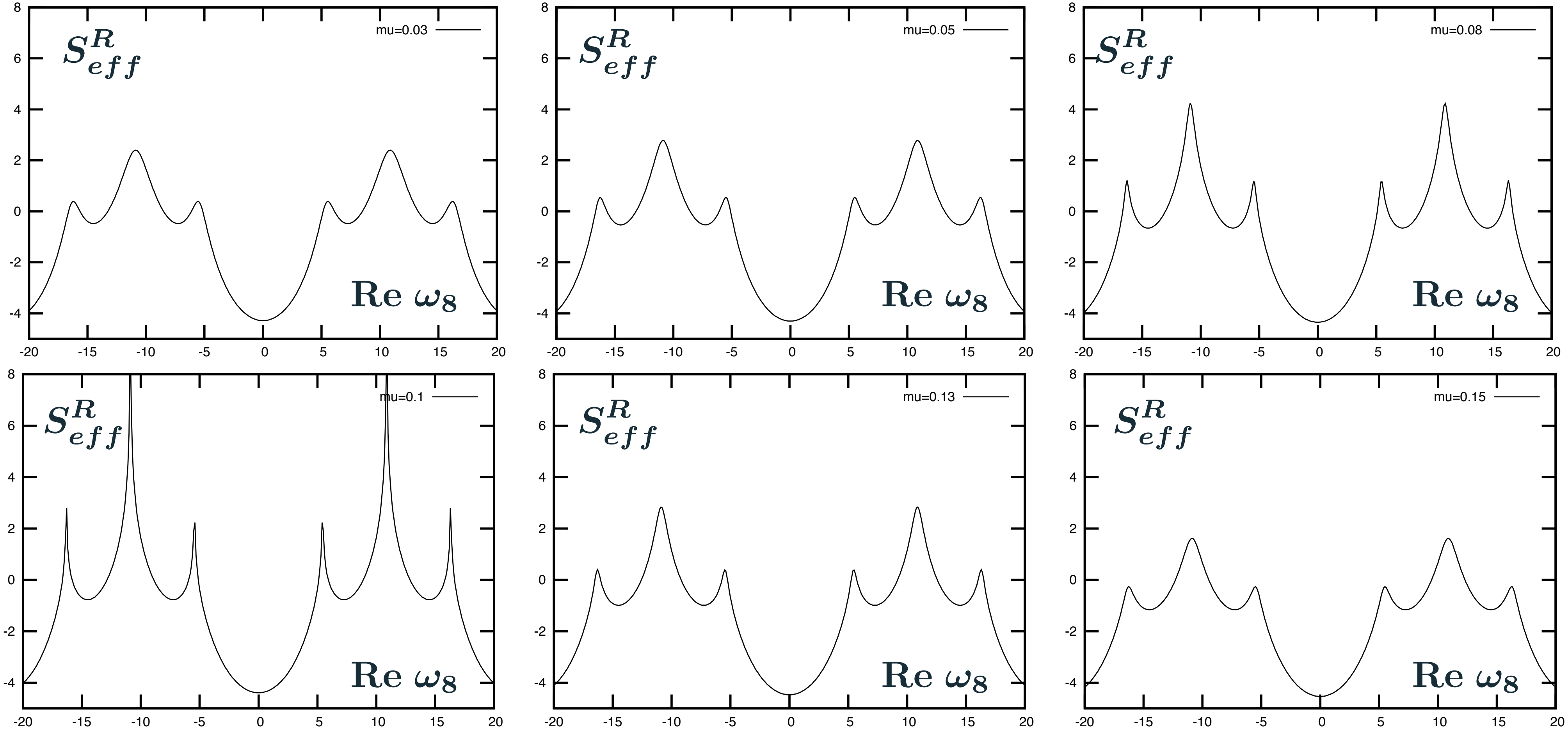
fist step: find saddle points (now in 16 dim.)

$am = 0.1$



(0+1) dimensional QCD

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fist step: find saddle points (now in 16 dim.)

- find 3 thimbles, related to Z(3) symmetry
- at $m = 0$, the thimbles are separated by singular points
- at $m = \mu_c$, the thimbles are separated by singular points
- saddle points are not μ-dependent

second step: diagonalize the hessian

$$\partial_a \partial_b S^R_{eff} = \mathrm{Tr}\left[D^{-1}\partial_a\partial_b D\right] - \mathrm{Tr}\left[D^{-1}(\partial_a D)D^{-1}(\partial_b D)\right]$$

- implementation is work in progress ...

Summary

- still many open question in the Lefschetz thimble approach that need to be clarified before it can be applied to full QCD
- (0+1) dimensional QCD is doable (at least in the reduced case)
- (n+1) dimensional QCD will be the next

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