

# Simulating low dimensional finite density QCD on Lefschetz Thimbles

Felix Ziesché

Physics Department  
Bielefeld University

Hadron Structure, Hadronic Matter, and Lattice QCD, Dubna 2017

# Motivation: The sign problem

For example in Lattice QCD with  $\mu > 0$ :  $S = S_R + iS_I \in \mathbb{C}$ .

$\rightarrow \frac{e^{-S}}{\int_{\Gamma} dU e^{-S}}$  is no probability density anymore.

Possible solution: Use the phase quenched partition sum

$Z_{pq} = \int_{\Gamma} dU e^{-S_R}$  and reweight with the phase:

$$\langle \mathcal{O} \rangle = \frac{\int dU \mathcal{O}(U) e^{-iS_I[U]} e^{-S_R[U]}}{\int dU e^{-S_R[U]}} \frac{\int dU e^{-S_R[U]}}{\int dU e^{-iS_I[U]} e^{-S_R[U]}} = \frac{\langle \mathcal{O} e^{-iS_I} \rangle_{pq}}{\langle e^{-iS_I} \rangle_{pq}}$$

How does  $\langle e^{-iS_I} \rangle_{pq}$  behave? Observe

- $\langle e^{-iS_I} \rangle_{pq} = \frac{Z}{Z_{pq}}$
- $Z_{pq} > Z \Rightarrow f - f_{pq} = \Delta f = -\frac{T}{V} \log \frac{Z}{Z_{pq}} > 0$   
 $\Rightarrow \langle e^{-iS_I} \rangle_{pq} = e^{-\frac{V}{T} \Delta f}$

Solution: Changing the integration contour to something that has no sign problem.

# The model: One flavor 0+1d-QCD

One space-time dimension:  $F_{\mu\nu} = 0 \Rightarrow S_G = 0$ .

$\rightarrow S = S_F$  and the discretized staggered fermion action reads:

$$\hat{S}_F(\mu) = \frac{1}{2} \sum_{n=0}^{N_\tau-1} \bar{\chi}(n) \left( e^\mu U(n) \chi(n+1) - e^{-\mu} U^\dagger(n-1) \chi(n-1) + 2m \chi(n) \right)$$

Integrating out the fermion fields in the partition sum, we have

$$Z(N_\tau, \mu) = \int dU d\bar{\chi} d\chi e^{-\bar{\chi} M[U] \chi} = \int dU \det M[U]$$

This determinant can be reduced to

$$\det(M[U]) = \frac{1}{2^{3N_\tau}} \det \left( 2 \cosh(N_\tau \sinh^{-1}(m)) \mathbb{I} + e^{N_\tau \mu} P + e^{-N_\tau \mu} P^\dagger \right)$$
$$P = \prod_{n=0}^{N_\tau-1} U(n).$$

For  $\mu > 0$ , this is complex.

# The Monodromy theorem

## Theorem

- Let  $f : \tilde{\Gamma} \rightarrow \mathbb{C}$  be a holomorphic function on  $\tilde{\Gamma}$  and
- $\Gamma, \Gamma' \subset \tilde{\Gamma}$  be homotopic submanifolds of  $\tilde{\Gamma}$  ( $\Gamma \simeq \Gamma'$ ).

Then

$$\int_{\Gamma} dz f(z) = \int_{\Gamma'} dz f(z).$$

If we have  $F : \Gamma \rightarrow \Gamma'$ , then we can express

$$\int_{\Gamma'} dz f(z) = \int_{\Gamma} dz \det[dF] f(z).$$

We take  $\Gamma = \mathrm{SU}(3)$ , whose complexification is  $\tilde{\Gamma} = \mathrm{SL}(3, \mathbb{C})$ .

$S$  can be analytically continued into  $\mathrm{SL}(3, \mathbb{C})$  by replacing  $P^\dagger$  with  $P^{-1}$ .

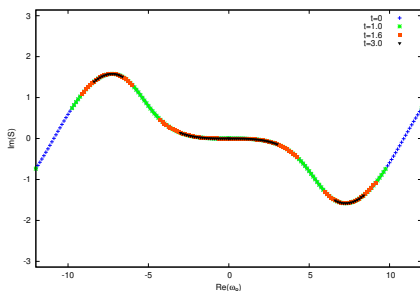
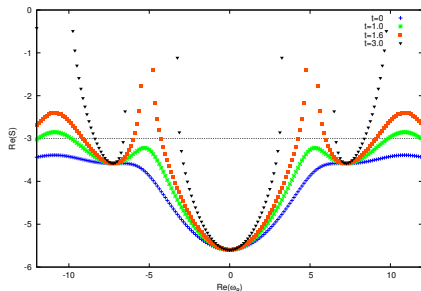
# Steepest ascent equation

$$\frac{d\omega_k}{dt} = \left( \frac{\partial S}{\partial \omega_k} \right)^* , \quad P(t) = \exp \left[ \sum_{k=1}^8 \omega_k(t) T^k \right]$$

- $S_I[P(t)] = \text{const.}$ , while  $S_R$  is increased.
- Induces Flow mapping for fixed  $t$

$$F_t: \text{SU}(3) \longrightarrow \mathcal{M}_t \subset \text{SL}(3, \mathbb{C})$$

$$P \longmapsto P(t) = e^{\sum_k \omega_k(t) T^k} .$$



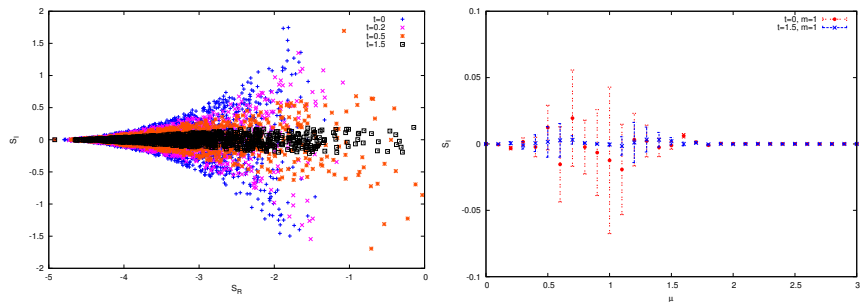
# The Contraction algorithm

A. Alexandru et al., Phys. Rev. D93, arXiv 1510.03258

- 1 Select starting point  $P_0 \in \text{SU}(3)$ .
- 2 Pick  $P_{n+1} \in \text{SU}(3)$  from an isotropic, ergodic distrib. around  $P_n$
- 3 Calculate  $\tilde{P}_{n+1} = F_t(P_{n+1})$  by integrating numerically (e.g. Runge Kutta)
- 4 Parallel transport  $e^1, \dots, e^8$  along  $F_t$  by integrating 
$$\frac{dv_k}{dt} = \left( \sum_{l=1}^8 \frac{\partial^2 S}{\partial \omega_k \partial \omega_l} v_l \right)^*$$
,  $\Rightarrow \det[dF_t] = \det[v^1(t), \dots, v^8(t)]$ .
- 5 Calculate  $S_{\text{eff}} = S_R - \log |\det[dF_t]|$
- 6 Accept  $\tilde{P}_{n+1}$  with probability  $\min\{1, e^{-(S_{\text{eff}}(\tilde{P}_{n+1}) - S_{\text{eff}}(\tilde{P}_n))}\}$ , otherwise  $P_{n+1} = P_n$  and repeat from 2.

$$\Rightarrow \langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} \frac{\det[dF_t]}{|\det[dF_t]|} e^{-iS_I} \rangle_{S_{\text{eff}}}}{\langle \frac{\det[dF_t]}{|\det[dF_t]|} e^{-iS_I} \rangle_{S_{\text{eff}}}}$$

# Comparison to Reweighting



**Figure:** Scatterplot of sampled configurations for  $m = 0.1, \mu = 0.35$  and the variations of  $S_I$  for  $t = 1.5$  and  $m = 1$  compared with normal Reweighting.

# Results for $m=1$

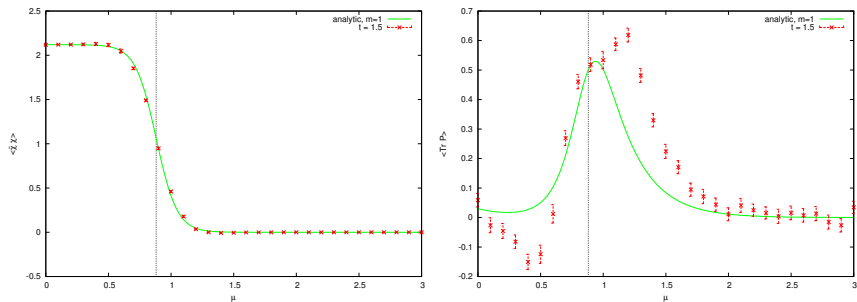


Figure: Results for  $N_\tau = 4, m = 1.0$  using the effective action.

More sophisticated approach needed.



F. Pham, *Proc. Symp. in Pure Math. Vol. 40* 319-333, 1983

$$Z = \int_{\text{SU}(3)} dP e^{-S}$$

- $S$  has only non-degenerate crit. points:

$$\frac{\partial S}{\partial \omega_k}(P_\sigma) = 0 \quad \forall k, \quad \det \left[ \frac{\partial^2 S}{\partial \omega_k \partial \omega_l} \right] (P_\sigma) \neq 0$$

- $\Rightarrow$  Lefschetz thimbles

$$\mathcal{J}_\sigma = \{P \in \text{SL}(3, \mathbb{C}) \mid F_t(P) \xrightarrow{t \rightarrow -\infty} P_\sigma\}$$

- $S|_{\mathcal{J}_\sigma} = \text{const.}$

$$\Rightarrow \text{SU}(3) \simeq \sum_{\sigma} n_{\sigma} \mathcal{J}_{\sigma}$$

$$\longrightarrow \int_{\text{SU}(3)} dP e^{-S} = \sum_{\sigma} n_{\sigma} e^{-iS_I[P_{\sigma}]} \int_{\mathcal{J}_{\sigma}} dP e^{-S_R}$$

# The geometric structure of 0+1d-QCD

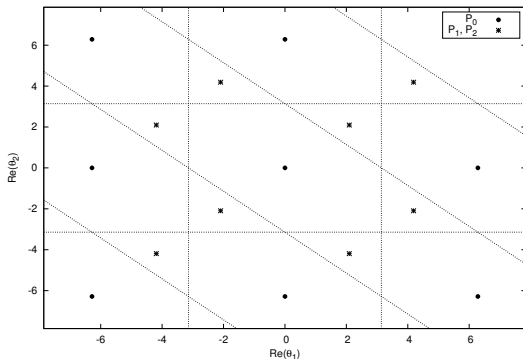
C. Schmidt and F. Ziesché, Proc. LATTICE2016, arXiv 1701.08959

- The critical points obtained are

$$P_\sigma = \mathbb{I}, e^{\pm i \frac{2\pi}{3}} \mathbb{I}.$$

These are the center elements of  $SU(3)$ . This is the original integration domain, so they all have intersection number  $n_\sigma = 1$ .

Including the divergent regions, where the thimbles end, we have:



# Which one contributes where... an approximation

The decomposition of the partition sum is

$$Z = \int_{\text{SU}(3)} dP e^{-S[P]} = \sum_{\sigma=0}^2 \int_{\mathcal{J}_k} dP e^{-S[P]} := \sum_{\sigma=0}^2 Z_{\sigma}$$

$Z_{\sigma}$  cannot be calculated directly by Monte Carlo. But at least, we want to know how much each partition sum contributes.

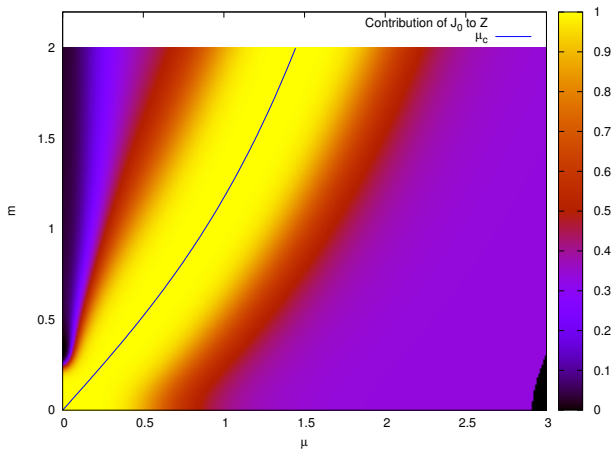
→ We approximate  $S$  around its critical points to get an estimate (Di Renzo, Erucci - Gaussian Approximation - see Lattice 2016):

$$S[P] \approx S[P_{\sigma}] + \frac{1}{2} \sum_{k,l} \left. \frac{\partial^2 S}{\partial \omega_k \partial \omega_l} \right|_{P_{\sigma}} (\omega_k(P) - \omega_k(P_{\sigma})) (\omega_l(P) - \omega_l(P_{\sigma}))$$

$$\Rightarrow Z \approx \sum_{\sigma=0}^2 \int \prod_{k=1}^8 d\omega_k e^{-S[P_{\sigma}] - \frac{1}{2} \sum_k \left. \frac{\partial^2 S}{\partial \omega_k \partial \omega_k} \right|_{P_{\sigma}} \omega_k^2}$$

# Which one contributes where... an approximation

We can now plot the ratio of  $|Z_0|$  over the overall sum.



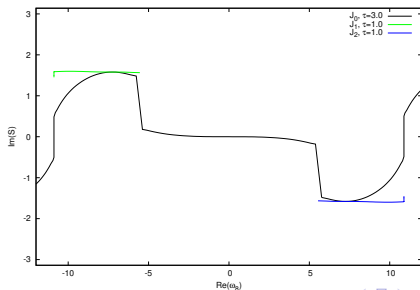
$$\frac{|Z_0|}{\sum_{\sigma} |Z_{\sigma}|}$$

# Metropolis on LTs

A. Mukherjee, *Phys. Rev. D*88, arXiv 1308.0233

- 1 Choose  $\mathcal{J}_\sigma$  with probability  $\frac{n_\sigma}{\sum_{\sigma'} n_{\sigma'}}$ .
- 2 Apply Steps 2 to 4 from Contraction algorithm with  $P_n \in T_{P_\sigma} \mathcal{J}_\sigma$  and  $(e^1, \dots, e^8)$  Basis of  $T_{P_\sigma} \mathcal{J}_\sigma$ . (One can get these by solving the Takagi eigeneq.)
- 3 Accept  $\tilde{P}_n$  with probability  $\min\{1, e^{-(S_{\text{eff}}(\tilde{P}_{n+1}) - S_{\text{eff}}(\tilde{P}_n))}\}$  and repeat from 1.

Flowtime  $t_\sigma$  and proposal width  $d_\sigma$  have to be tuned according to the Thimble.



- Improvement of Maryland Approach: Parallel Tempering (see e.g. *A. Alexandru et al. 1703.02414*, *M. Fukuma et al. 1703.00861*)
- higher-dimensional Lattice-QCD: Critical points  $\rightarrow$  Gauge Orbits  $\Rightarrow$  Generalized Lefschetz thimbles (see *E. Witten 1001.2933*)
- Applications to other sign problems (e.g. Real-Time QCD)
- Usage in continuum theory (Resurgence theory, instantons, ...)

# The Hessian $\partial^2 S$

To calculate the Takagi vectors, which span the tangent space  $T_{P_\sigma} \mathcal{J}_\sigma$ , we need to calculate the Hessian

$$\frac{\partial^2 S}{\partial \omega_k \partial \omega_l} = \text{Tr} \left[ M^{-1} \frac{\partial M}{\partial \omega_k} M^{-1} \frac{\partial M}{\partial \omega_l} - M^{-1} \frac{\partial^2 M}{\partial \omega_k \partial \omega_l} \right].$$

... which is easy for  $P = e^{i\gamma} \mathbb{I}$

$$\frac{\partial^2 S}{\partial \omega_k \partial \omega_l} = \frac{1}{2} \left( \frac{\cosh(N_\tau \mu + i\gamma)}{B_\gamma} - \frac{\sinh^2(N_\tau \mu + i\gamma)}{B_\gamma^2} \right) \delta^{kl} =: h_\gamma \delta^{kl}$$

with

$$B_\gamma = \cosh(N_\tau \mu c) + \cosh(N_\tau \mu + i\gamma).$$

The Takagi equation reads

$$H^* \rho_\lambda^* = \lambda \rho_\lambda, \quad \lambda \in \mathbb{R}$$

... with  $H^{kl} = h_\gamma \delta^{kl}$ , we have as solutions

$$\lambda = |h_\gamma|, \quad \rho_\lambda^k = c e^k \quad \text{with} \quad c = \sqrt{\frac{h_\gamma^*}{|h_\gamma|}}.$$