Thimbles and Lattice Gauge Theories

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SIGN 2018, Bielefeld, September 11, 2018

11.09.2018

A short introduction to Morse theory

CRC-TR 211

- Let M be a smooth compact m-dimensional mainfold,
- $f : M \to \mathbb{R}$ a at least two times differentibale function.
- $p \in M$ is called a non-degenrate *critical point* of f, if $\nabla f(p) = 0$ and $\det \nabla^2 f(p) \neq 0$.
- $\to M^a := \{p \in M | f(p) \leq a\} = f^{-1}((-\infty, a])$ is compact, since M is compact.

$\Rightarrow M$ has the homotopy type of a CW-complex, where each cell is related to a non-degenerate critical points. Its dimension is the number of positive eigenvalues of $\nabla^2 f$. A *CW-complex* is a cell-complex, where a k-cell is a closed disc

$$D^k = \{\vec{x} \in \mathbb{R}^k | \, |\vec{x}| \leq 1\},$$

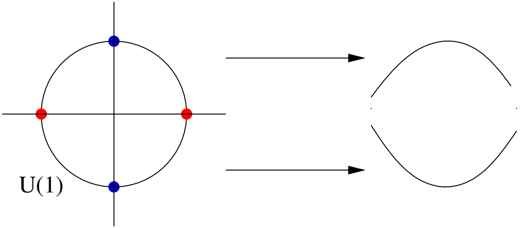
which are glued together at the boundaries to form a compact manifold.

An example

$$f(z) = \mathrm{Re}\,(z^2 - 1), \quad z \in \mathrm{U}(1)$$

- f has four critical points $z = 1, -1, i, -i$.
- $\partial_z^2 f(z) > 0$ for $z = i, -i$ at $f = -2$ and $\partial_z^2 f(z) < 0$ for $z = 1, -1$ at $f = 0$

$\Rightarrow$ We have two 1-cells glued together at two 0-cells.



In complexified space, these cells can be chosen to have constant phase and are then called *Lefschetz thimbles*.

The Lefschetz theorem

A complex analytic manifold M of complex dimension k, bianalytically embedded as a closed subset of $\mathbb{C}^n$ has the homotopy type of a k-dimensional CW-complex.

This means, that every Lefschetz thimble has the same dimension.

The Monodromy theorem

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

Then

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

The model: One flavor 0+1d-QCD

One space-time dimension: $F_{\mu\nu} = 0 \Rightarrow S_G = 0$.
$\longrightarrow S = S_F$ and the discretized staggered fermion action reads:

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

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

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

This determinant can be reduced to

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

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

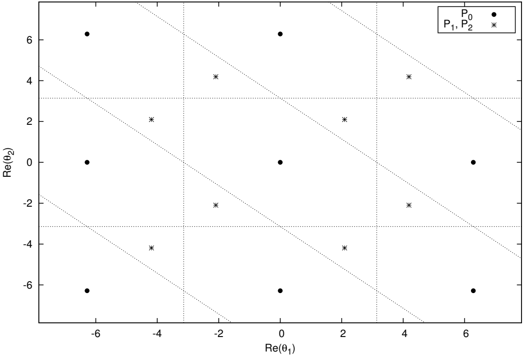
C. Schmidt and F. Ziesché, Proc. LATTICE2016, arXiv 1701.08959

- The main 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).

Including zeros of $\det[M]$, we have:



The triangulation approach

1. Get the relevant saddle-point/thimble structure. (Done for 1d-QCD)
2. Solve the flow equations for specific directions around the saddle points and record the points with a minimum curvature.
3. With these points, we construct a mesh of d-simplices, which approximates the thimbles.
4. Do an ergodic MCMC on this mesh.

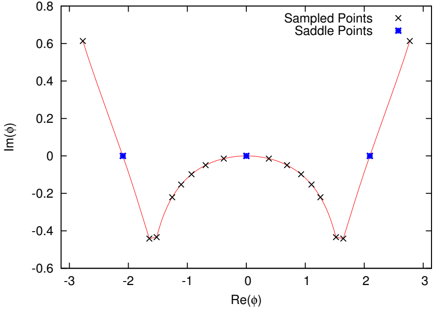
Advantages:

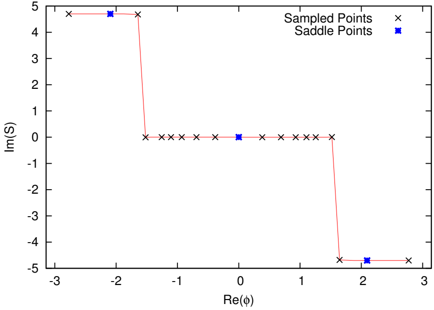
- The Monodromy Theorem is fulfilled $\Rightarrow$ No a priori wrong results.
- Sampling on a mesh is fast!

Sampling the points

1. Start at a saddle point.
2. Go an ϵ-step in direction of the Takagi-Vectors defined by
$$H(\omega_\sigma)^*\hat{\omega}_\sigma^* = \lambda\hat{\omega}_\sigma, \quad \lambda \in \mathbb{R}$$
3. The steepest ascent equation can be reformulated to
$$\dot{\omega} = \left(\frac{\partial S}{\partial \omega}\right)^* \Rightarrow \dot{\omega}_R = \frac{\partial S_I}{\partial \omega_I} \text{ and } \dot{\omega}_I = -\frac{\partial S_I}{\partial \omega_R}.$$
This can be solved effectively by symplectic methods. We use Verlet-integration.
4. Flow until you hit $|\nabla S| < \epsilon$ or $S \geq S_{\mathrm{CutOff}}$ and record the points.
5. Reduce the number of points depending on a maximal discrete curvature.

Sampling the points





The recorded points in ω_8-direction and the corresponding imaginary part of the action.

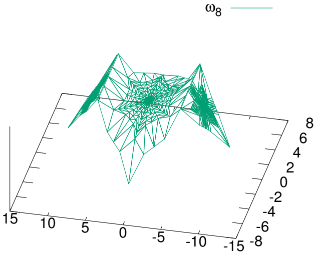
Building the triangulation

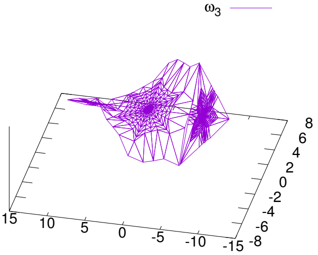
We take two neighboring flowlines consisting of the points $\{p_1^0, p_1^1, p_1^2, \ldots\}$ and $\{p_2^0, p_2^1, p_2^2, \ldots\}$, where $p_1^0 = p_2^0$ is the common critical point. We connect both flowlines for themselves and define $\tilde{l}_i^k := l_i^k / L_i$ to be the normalised distance to the critical point.

1. Start with $m_1 = m_2 = 1$.
2. Connect $p_1^{m_1}$ with $p_2^{m_2}$.
3. If $\sum_{k=1}^{m_2} \tilde{l}_k^2$ is smaller than $\sum_{j=1}^{m_1} \tilde{l}_j^1$, increment m_2 or vice versa and go back to step 2.
4. When one of the m_i's reaches n_i, leave it there and just increment the other one and connect them until this reaches the end, too.

This procedure is generalisable for higher dimensions!

$$\text{Triangles} \to n\text{-simplices.}$$





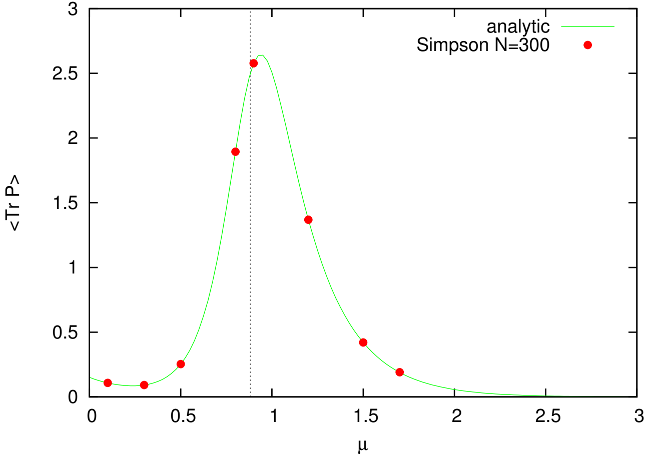
Triangulation in ω_8 and ω_3 direction at $N_\tau = 4$ and $m = 1.0$ at $\mu = 0.5$.

Sampling the triangulation (RW-Slice Sampling)

1. Select starting point P_0 on the triangulation.
2. Pick a random number $u \in [\exp(-S_{\mathrm{CutOff}}), \exp(-S_R(F_t(P_n)))]$ uniformly.
3. Pick P_{n+1} from an isotropic, ergodic distrib. around P_n on the triangulation.
4. Accept P_{n+1}, if $\exp(-S_R(\tilde{P}_{n+1})) > u$. Otherwise $P_n = P_{n+1}$ and repeat from 3.

This obviously can be improved by using a more heatbath-like update, but this has at least no ergodicity problems.
The *walking* on the triangulation is still to be implemented. So we have Results just for the ω_8-direction.

Results (at least for ω_8)



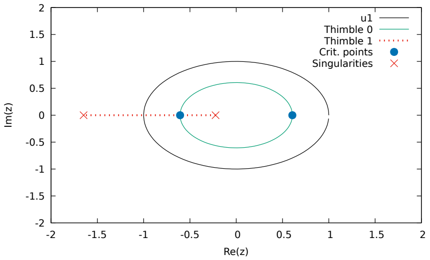
The Polyakov Loop for $N_\tau = 4$, $m = 1.0$.

A simple U(1)-integral

$$f(U) = 2\cosh(K_c) + e^K U + e^{-K} U^{-1}, \quad U \in \mathrm{U}(1)$$

$$Z = \int_{\mathrm{U}(1)} \mathrm{d}U f(U) = \int_0^{2\pi} \frac{\mathrm{d}\phi}{2\pi} f(e^{i\phi}) = \int_{B_1(0)} \frac{\mathrm{d}z}{2\pi i} \frac{f(z)}{z}$$

- Residual theorem: $Z = 2\cosh(K_c)$ and $< e^{i\phi} >= \frac{e^{-K}}{2\cosh(K_c)}$
- $S = -\log f(z) \longrightarrow z_c = \pm e^{-K}$ and poles at $z = -e^{-K \pm K_c}$.



Now, what if we have more links?

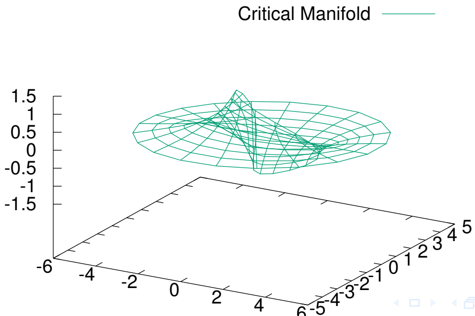
Gauge orbits

$$f(U_1, U_2) = 2\cosh(K_c) + e^K U_1 U_2 + e^{-K} U_2^{-1} U_1^{-1}, \quad U \in \mathrm{U}(1)$$

- The critical equation goes to

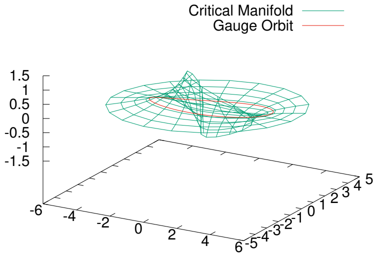
$$e^{i(\phi_1+\phi_2)} = \pm e^{-K} \Rightarrow \ \phi_1^R + \phi_2^R = 0/\pi \mod 2\pi, \ \ \phi_1^I + \phi_2^I = K$$

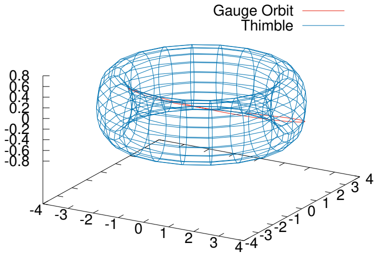
- So we have two 2-dimensional critical manifolds.



Gauge orbits

According to Witten, we have to take a cycle on this critical manifold and then sample from that cycle up to the so-called generalized Lefschetz thimble.





Outlook

- Extending the simulations from 0+1d-QCD to 1+1d-QCD, by using Lattice symmetries.
- Explore the relationship between Lattice symmetries and thimble structure in general (Test case: 1+1d-Quenched QED).
- Find an effective way of dealing with gauge orbits (Promising work in progress ;-))
- Complete the sampling on triangulations and implement for higher dimensions.

Thank you for your attention!

Projection of $\mathbb{C}^2$ onto $\mathbb{R}^3$

$$
\begin{aligned}
x &= \left(r_1 e^{-\mathrm{Im}\,(\phi_1)} + r_2 e^{-\mathrm{Im}\,(\phi_1)} \cos(\mathrm{Re}\,(\phi_2))\right) \cos(\mathrm{Re}\,(\phi_1)) \\
y &= \left(r_1 e^{-\mathrm{Im}\,(\phi_1)} + r_2 e^{-\mathrm{Im}\,(\phi_1)} \cos(\mathrm{Re}\,(\phi_2))\right) \sin(\mathrm{Re}\,(\phi_1)) \\
z &= r_2 e^{-\mathrm{Im}\,(\phi_2)} \sin(\mathrm{Re}\,(\phi_2))
\end{aligned}
$$