Simulating gauge theories on Lefschetz thimbles

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Lattice 2019, Wuhan

June 18, 2019

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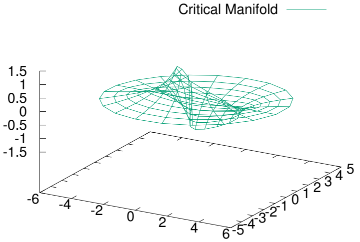
In full Lattice Gauge Theories new problems arise:

- Gauge and Lattice symmetries
  $\rightarrow$ Critical manifolds intead of critical points
  $\longrightarrow$ Traditional Picard-Lefschetz theory does not apply anymore.
- High dimensionality.



Crit. manifold of a $\mathrm{U}(1)$*-2-link model.*

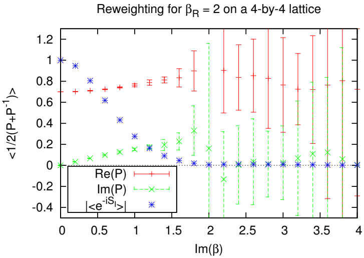
- We apply the concept of Generalized Lefschetz Thimbles (*E. Witten, arXiv 1001.2933*)
- More freedom gives us more tools.

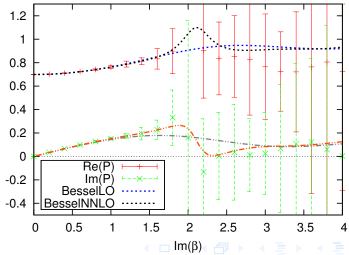
Pure 1+1d-U(1)-YangMills @ complex β

$$S[U] = \beta \sum_x \left[1 - \frac{1}{2}(P_x + P_x^{-1}) \right], \quad P_x = U_0(x) U_1(x+\hat{0}) U_0^{-1}(x+\hat{1}) U_1^{-1}(x)$$

- For $\beta_I > 0$, there's a sign problem.
- We have a formal solution for comparison.

$$Z(\beta) = \sum_{n=-\infty}^{+\infty} [I_n(\beta)]^V$$



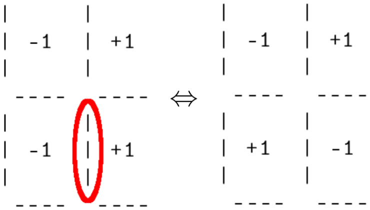


Critical manifolds

- The critical manifolds ($\nabla S = 0$) are characterized by

$$P_x = P_{x+\hat{\mu}} \text{ or } P_x = -P^{-1}_{x+\hat{\mu}},\ \mu \in \{0,1\} \ \text{ and } \ \prod_x P_x = 1.$$

- Choose: $P_x = \pm 1$ and only an even number of $P_x = -1$.
- Observe: Critical configurations with $0 < \#\{P_x = -1\} < V$ get additional zero modes.
  $\rightarrow$ Only $\#\{P_x = -1\}$ is relevant, not their position.
  $\longrightarrow$ We have $(\lfloor \frac{V}{2} \rfloor + 1)$ crit. manifolds with different S_I.



Leading order approximation and expansion

- Removing PBCs leads to the LO approximation

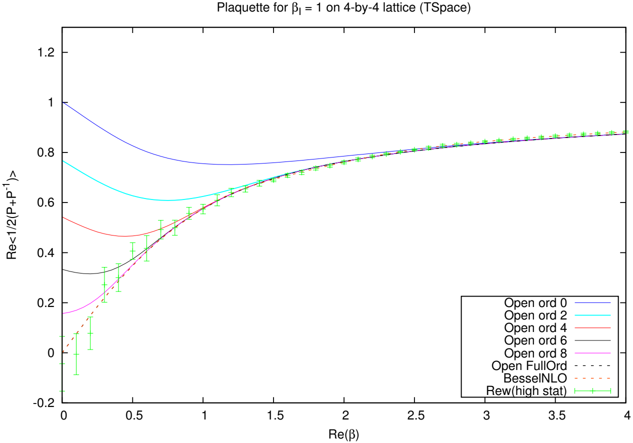
$$Z = \left[\int_{\mathrm{U}(1)} \mathrm{d}P e^{\beta/2(P+P^{-1})}\right]^V = [I_0(\beta)]^V .$$

- Crit. points are at $P = \pm 1$. Expansion in thimbles $\mathcal{J}_0, \mathcal{J}_1$:

$$\begin{aligned} Z &= \left[\int_{\mathcal{J}_0} \mathrm{d}P e^{\beta/2(P+P^{-1})} + \int_{\mathcal{J}_1} \mathrm{d}P e^{\beta/2(P+P^{-1})}\right]^V =: [Z_0 + Z_1]^V \\ &= \sum_{k=0}^{V} \binom{V}{k} Z_0^{V-k} Z_1^k . \end{aligned}$$

- Every even term corresponds to a thimble on the original model
  $\Rightarrow$ Gives a hint for their importance.

Hierarchy of thimbles

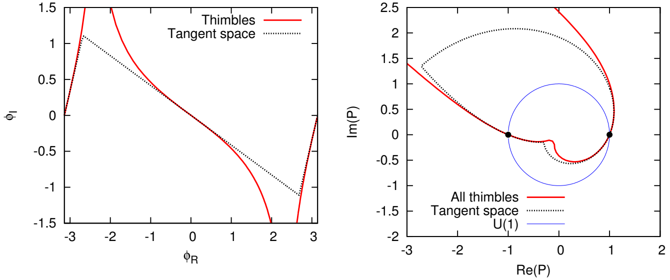


The crit. manifolds form a hierarchy with different phases and importance

$$e^{-iS_I} = e^{-i4k\beta_I}, \;\; e^{-S_R} = e^{-i4k\beta_R}, \; k = 0, \ldots, \lfloor \frac{V}{2} \rfloor .$$

Motivation for tangential manifolds

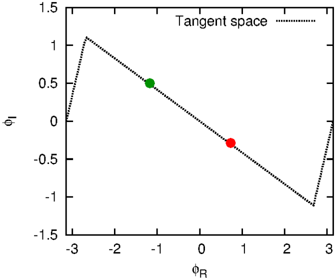
Local thimbles can be calculated for single plaquettes:



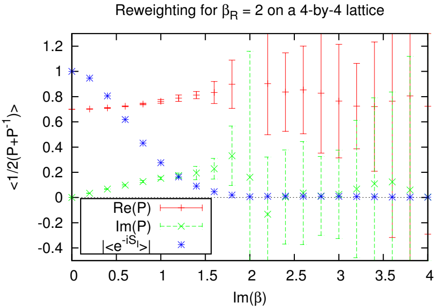
- Tangential manifolds are close to the thimbles in the most important regions.
- Their union is still homotopic to $\mathrm{U}(1)$.
- A local sampling algorithm can be implemented.

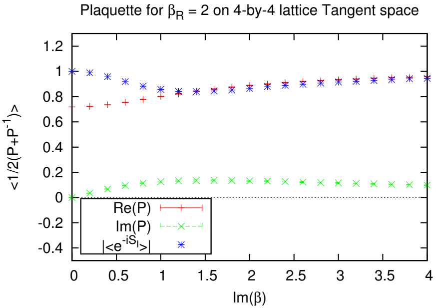
Metropolis on Main tangent space

1. Take the tangent space for single plaquettes.
2. Update the links, so the neighboring plaquettes stay on the main tangent space.
3. If the proposal drives one plaquette out of the tangential manifold, reject the configuration (Zero probability).

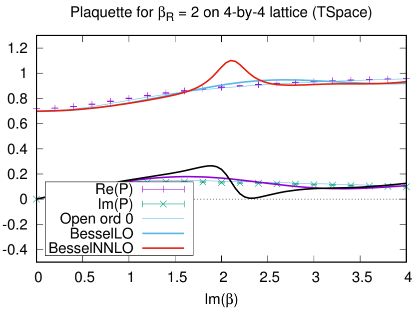


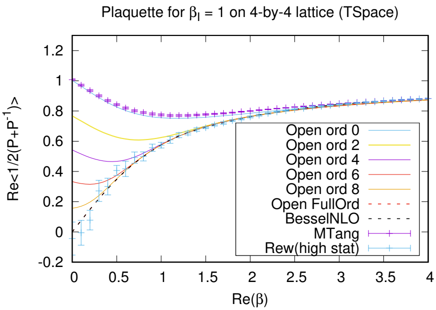
Results





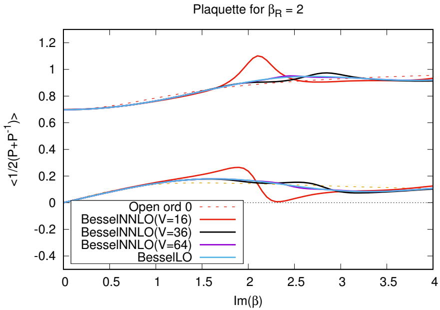
Plaquette for $\beta_R = 2$ with Reweighting and on the main tangential manifold on a 4-by-4 lattice.

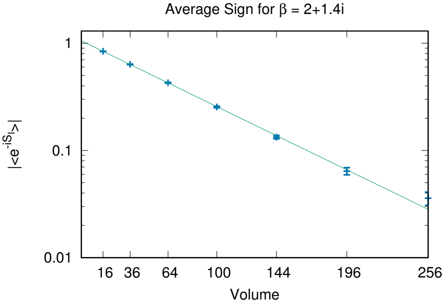




Comparison with approximation for constant $\beta_R = 2$ and $\beta_I = 1$.

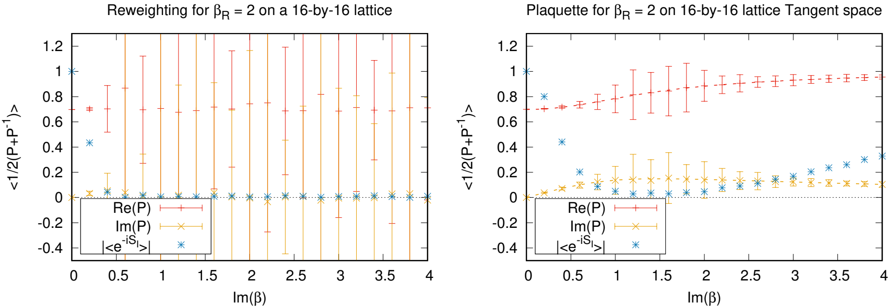
Volume dependence





Volume dependence of the formal solution and the average sign of the main tangential manifold.

Results for V = 256



Plaquette for $\beta_R = 2$ with Reweighting and on the main tangential manifold on a 16-by-16 lattice.

Reweighting to subleading tangential man.

CRC-TR 211

S. Bluecher et al., PoS LATTICE **2018** *(2019), arXiv 1901.05187*
For taking another thimble or tang. man. τ_1 into account, we need the ratio Z_1/Z_0. Suppose, we have a mapping

$$f : \tau_0 \longrightarrow \tau_1 .$$

Then we can write

$$\frac{Z_1}{Z_0} = \frac{\int_{\tau_0} \mathrm{d}U e^{-S[f(U)]+S[U]} \det[\mathrm{d}f] e^{-S[U]}}{\int_{\tau_0} \mathrm{d}U e^{-S[U]}} = < e^{-S\circ f+S} \det[\mathrm{d}f] >_0$$

- The difficulty is to find a suitable f.
- For tangent spaces, f is linear.
  $\Rightarrow$ $\det[\mathrm{d}f]$ will be a constant factor.

Outlook

- Implementation of the reweighting is going on.
- Structure for non-abelian Lie groups ($\mathrm{SU}(2)$, $\mathrm{SU}(3)$).
- Generalization to 2+1d, 3+1d.
- Including the fermion matrix at complex β.
- Including chemical potential μ for $\mathrm{SU}(3)$
  $\longrightarrow$ see also the Talk by Yuto Mori.

Thank you for your attention!

But this is not always the case:

For $\mu > 0$: $S = S_R + iS_I \in \mathbb{C}$.
$\rightarrow \frac{e^{-S}}{\int_\Gamma \mathrm{d}Ue^{-S}}$ is no probability density anymore $\rightarrow$ No MCMC.
Possible solution: Use the phase quenched partition sum $Z_{pq} = \int_\Gamma \mathrm{d}Ue^{-S_R}$ and reweight with the phase:

$$< \mathcal{O} >= \frac{\int \mathrm{d}U\mathcal{O}(U)e^{-iS_I[U]}e^{-S_R[U]}}{\int \mathrm{d}Ue^{-S_R[U]}} \frac{\int \mathrm{d}Ue^{-S_R[U]}}{\int \mathrm{d}Ue^{-iS_I[U]}e^{-S_R[U]}} = \frac{< \mathcal{O}e^{-iS_I} >_{pq}}{< e^{-iS_I} >_{pq}}$$

How does $< e^{-iS_I} >_{pq}$ behave? Observe

- $< e^{-iS_I} >_{pq} = \frac{Z}{Z_{pq}}$
- $Z_{pq} > Z \;\Rightarrow\; f - f_{pq} = \Delta f = -\frac{T}{V} \log \frac{Z}{Z_{pq}} > 0.$

$$\Rightarrow < e^{-iS_I} >_{pq} = e^{-\frac{V}{T}\Delta f}$$

The idea

- We complexify the d.o.f. and analytically continue e^{-S} and $\mathcal{O}$.
- Observe: e^{-S} and $\mathcal{O}$ are holomorphic functions in some area.
  $\rightarrow$ Choosing a homotopic integration contour in that area gives the same result for $< \mathcal{O} >$. (Monodromy/Cauchy's Theorem)
- But that's not true for e^{-iS_I} and e^{-S_R}!
  $\rightarrow < e^{-iS_I} >$ depends on the integration contour.

We will use Picard-Lefschetz theory (a complex version of Morse theory) to find a good contour!

A short introduction to Morse theory

- Let M be a smooth compact m-dimensional manifold,
- $f : M \to \mathbb{R}$ a at least two times differentiable function, so that
- f has only non-degenerate critical points (this is $p \in M$ with $\nabla f(p) = 0$ and $\det \nabla^2 f(p) \neq 0$).

$\Rightarrow$ M has the homotopy type of a cell-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 k-cell is an open disc

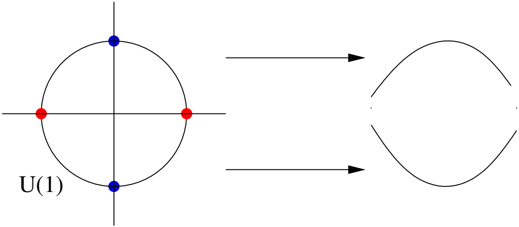
$$D^k = \{\vec{x} \in \mathbb{R}^k |\ |\vec{x}| < 1\},$$

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

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

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

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



In complexified space, these cells can be chosen to conserve the imaginary part of our action and are then called *Lefschetz thimbles*.

Steepest ascent/descent equation

$$\frac{\mathrm{d}z}{\mathrm{d}t} = \pm \left(\frac{\partial S}{\partial z}\right)^* = \pm \frac{\partial S_R}{\partial z_R} \pm i \frac{\partial S_R}{\partial z_I}$$

- $S_I[P(t)] = \mathrm{const.}$, while S_R is increased/decreased.
- Solution of steepest ascent eq. for fixed t will be called Flow mapping

$$\begin{aligned} F_t : \mathbb{R} &\longrightarrow \mathcal{M}_t \subset \mathbb{C} \\ z(0) &\longmapsto z(t). \end{aligned}$$

$\longrightarrow$ No sign problem along solutions.

Lefschetz thimbles

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

$$Z = \int_{\mathbb{R}} \mathrm{d}z e^{-S(z)}$$

- S is locally holomorphic and has only non-degenerate crit. points: $\frac{\partial S}{\partial z}(z_\sigma) = 0$ and $\det\left[\frac{\partial^2 S}{\partial z^2}\right](z_\sigma) \neq 0$
- Definition of Lefschetz thimbles

$$\mathcal{J}_\sigma = \{z \in \mathbb{C} \mid F_t(z) \xrightarrow{t \to -\infty} z_\sigma\}$$

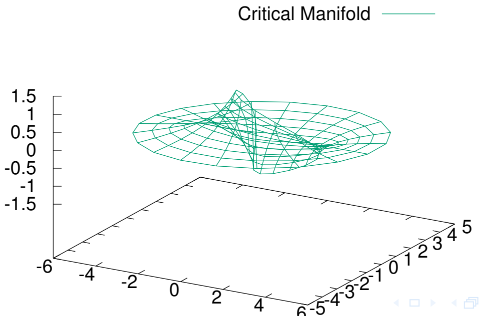
- We have $e^{-S_I}\big|_{\mathcal{J}_\sigma} = \mathrm{const.}$ and $\mathbb{R} \simeq \sum_\sigma n_\sigma \mathcal{J}_\sigma$, where $n_\sigma =< \mathcal{K}_\sigma, \mathbb{R} >$ is the so called Kronecker index.

$$\longrightarrow \int_{\mathbb{R}} \mathrm{d}z e^{-S} = \sum_\sigma n_\sigma e^{-iS_I[z_\sigma]} \int_{\mathcal{J}_\sigma} \mathrm{d}z e^{-S_R}$$

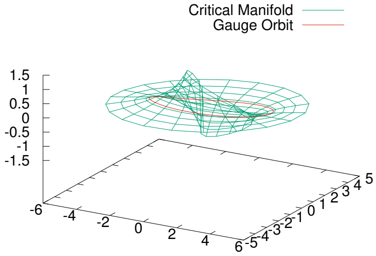
How can we do that practically?

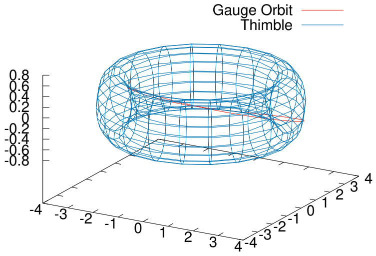
$$f(U_1, U_2) = 2\cosh(K_c) + e^K U_1 U_2 + e^{-K} U_2^{-1} U_1^{-1}, \quad U \in \mathrm{U}(1)$$

- The critical equation goes to
$$e^{i(\phi_1+\phi_2)} = \pm e^{-K} \Rightarrow \phi_1^R + \phi_2^R = 0/\pi \mod 2\pi, \quad \phi_1^I + \phi_2^I = K$$
- So we have two 2-dimensional critical manifolds.



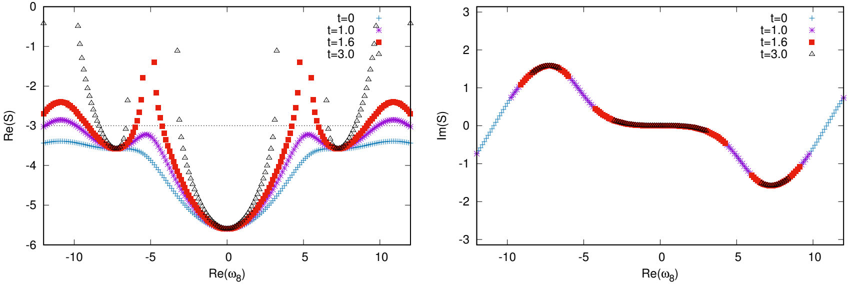
According to Witten, we have to take a cycle on this critical manifold and then solve the flow equations at each point of the cycle in the positive Takagi directions to get the generalized Lefschetz thimble.





A. Alexandru et al., Phys. Rev. D93, arXiv 1510.03258 and many more

- Idea: Take the original real manifold or a tangent space to the critical points and solve the steepest **ascent** equation for a finite time to flow near the thimbles.
- This effectively *contracts* the thimbles onto small neigborhoods around the critical points.
- Originally used together with a Metropolis algorithm.



Results for the Contraction Algorithm

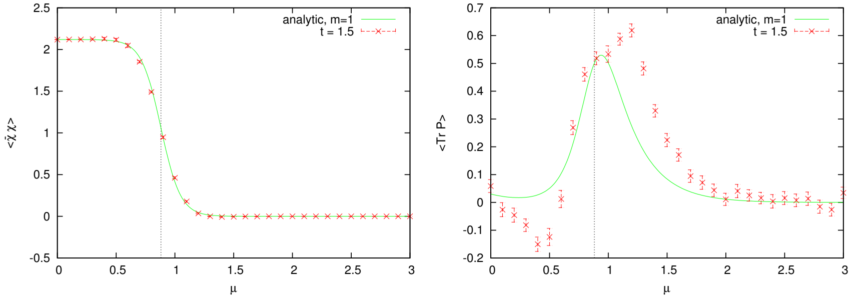


Figure: Results for $N_\tau = 4$, $m = 1.0$ using the effective action.

An ergodic sampling method: Slice Sampling

1. Select starting point P_0 on the triangulation.
2. Pick a random number $u \in [\exp(-S_{\mathrm{CutOff}}), \exp(-S_R(P_n))]$ uniformly.
3. Sample uniformly a point P_{n+1} from the set $\{P \in \mathrm{SU}(3) | e^{-S_R(P)} > u\}$.
4. Repeat from step 2 using the new P_{n+1}.

The problem is step 3. But for Thimbles, we know the approximate probability distribution!
$\rightarrow$ We can approximate it with a sharp gaussian distribution and use envelope/rejection sampling!

But for low-dimensional models, one can use a very easy way.

Sampling the triangulation (RW-Slice Sampling)

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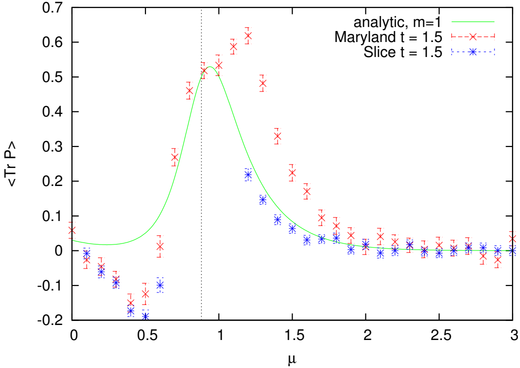
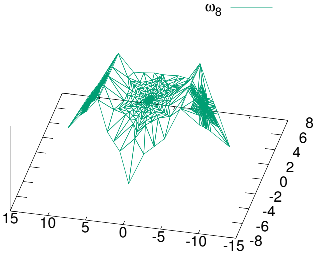
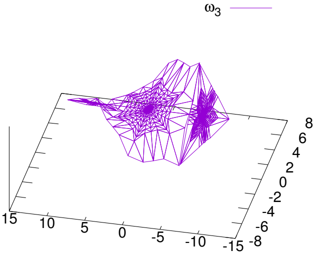
1. Select starting point P_0 on the triangulation.
2. Pick a random number $u \in [\exp(-S_{\mathrm{CutOff}}), \exp(-S_R(P_n))]$ uniformly.
3. Pick P_{n+1} from an isotropic, ergodic distrib. around P_n on the triangulation.
4. Accept P_{n+1}, if $\exp(-S_R(\tilde{P}_{n+1})) > u$. Otherwise $P_n = P_{n+1}$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

Contraction vs. Slice Sampling



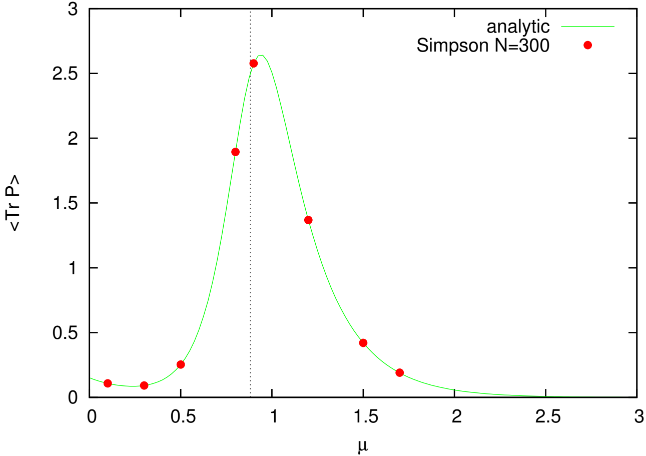
$\longrightarrow$ Better results for $\mu > \mu_c$, BUT same for $\mu < \mu_c$.





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

Results (at least for ω_8)



The Polyakov Loop for $N_\tau = 4, m = 1.0$. The method doesn't obviously show the problems of the holomorphic gradient flow.

Some Important theorems

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

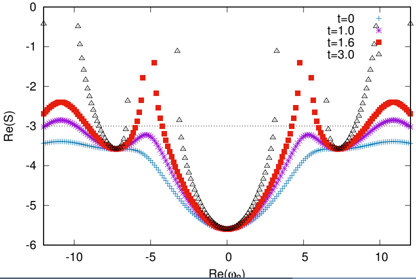
$$\int_\Gamma \mathrm{d}z f(z) = \int_{\Gamma'} \mathrm{d}z f(z).$$

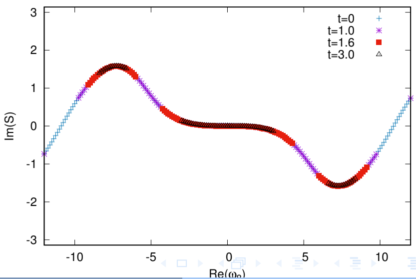
Steepest ascent equation

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

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

$$\begin{aligned} F_t : \mathrm{SU}(3) &\longrightarrow \mathcal{M}_t \subset \mathrm{SL}(3,\mathbb{C}) \\ P &\longmapsto P(t) = e^{\sum_k \omega_k(t) T^k}. \end{aligned}$$





The Contraction algorithm

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

1. Select starting point $P_0 \in \mathrm{SU}(3)$.
2. Pick $P_{n+1} \in \mathrm{SU}(3)$ 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 $e^1, \ldots, e^8$ along F_t by integrating $\frac{\mathrm{d}v_k}{\mathrm{d}t} = \left(\sum_{l=1}^{8} \frac{\partial^2 S}{\partial\omega_k \partial\omega_l} v_l\right)^*$, $\Rightarrow \det[\mathrm{d}F_t] = \det[v^1(t), \ldots, v^8(t)]$.
5. Calculate $S_{\text{eff}} = S_R - \log|\det[\mathrm{d}F_t]|$
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.

$$\Rightarrow < \mathcal{O} > = \frac{< \mathcal{O} \frac{\det[\mathrm{d}F_t]}{|\det[\mathrm{d}F_t]|} e^{-iS_I} >_{S_{\text{eff}}}}{< \frac{\det[\mathrm{d}F_t]}{|\det[\mathrm{d}F_t]|} e^{-iS_I} >_{S_{\text{eff}}}}$$

Effect of F_t on the simulation

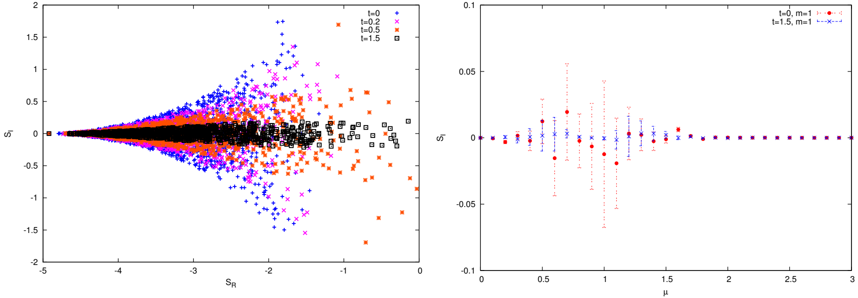


Figure: Scatterplot of sampled configurations for $m = 0.1, \mu = 0.35$ and the variations of S_I for $t = 1.5$ and $m = 1$ compared with normal Reweighting.

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

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