Lefschetz thimbles and Lattice gauge theories

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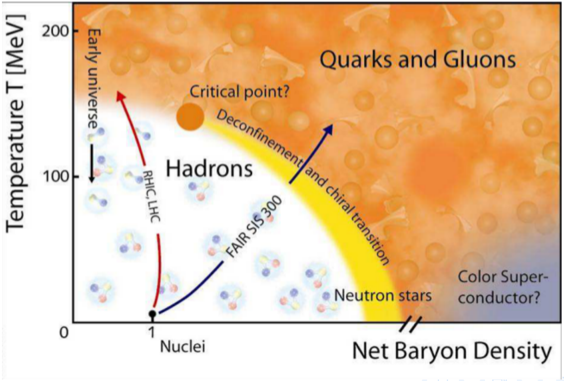
What do we want?

- Modern quantum field theories describe three of the four fundamental forces.
  1. The electromagnetic force → Quantum Electro Dynamics (QED)
  2. The weak nuclear force (together with the above)→ Electroweak theory
  3. The strong nuclear force → Quantum Chromo Dynamics (QCD)
- Our interest is the thermodynamics of the strong force (QCD)



From quantum to lattice field theory

- All thermodynamic observables can be calculated from the grand canonical partition sum

$$Z(T,\mu,V)=\int \mathrm{d}A_\nu \mathrm{d}\bar{\Psi}\mathrm{d}\Psi e^{-S^E[A_\nu,\bar{\Psi},\Psi,T,\mu,V]},$$

- The action of QCD is

$$\begin{aligned} S^E &= \int_0^{1/T}\mathrm{d}\tau\int_V \mathrm{d}^3x\frac{1}{4}F_{\alpha\beta}F_{\alpha\beta}+\sum_{f=1}^{N_f}\bar{\psi}^f(\gamma_\nu^E(\partial_\nu+ig_0A_\nu)+i\gamma_4^E\mu_f+m_f)\psi^f, \\ F_{\alpha\beta} &= \partial_\alpha A_\beta-\partial_\beta A_\alpha+ig_0[A_\alpha,A_\beta],\quad A_\nu\in i\mathfrak{su}(3). \end{aligned}$$

- Analytic evaluation of the functional integral is practically impossible.
- space-time $\rightarrow$ lattice, derivatives $\rightarrow$ finite differences:

$\Rightarrow$ quantum field theory $\longrightarrow$ lattice field theory

This can be simulated on computers via Markov Chain Monte Carlo!

Prerequisite: e^{-S^E} is a probability density.

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But this is not always the case:

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

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

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 $< \mathcal{O} >$.
- 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

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

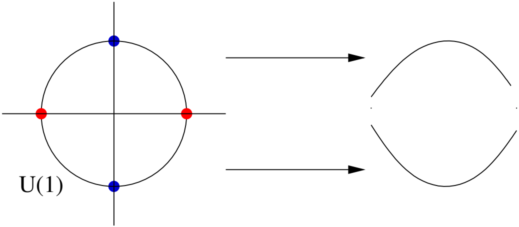
which are glued together at the boundaries to form a compact manifold.

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 $z = 1, -1$ 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 $e^{-S_I}\big|_{\mathcal{J}_\sigma} = \text{const.}$ and $\mathbb{R} \simeq \sum_\sigma n_\sigma \mathcal{J}_\sigma$, where $n_\sigma =< \mathcal{J}_\sigma, \mathbb{R} >$ 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?

The triangulation approach

1. Get the relevant saddle-point/thimble structure.
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!

The model: One flavor 0+1d-QCD

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

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

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

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

This determinant can be reduced to

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

$$P = \prod_{n=0}^{N_\tau - 1} U(n).$$

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

Complexification

- We use the representation of the SU(3)-matrices P as exponentials of Gell-Mann-Matrices

$$P = \exp\left[\sum_{k=1}^{8} \omega_k T^k\right] \quad T^k = -\frac{i}{2}\lambda^k \; k = 1\dots 8$$

- For $\omega_k \in \mathbb{R}$, P is in SU(3) and $P^\dagger = P^{-1}$.
- For Applying Picard-Lefschetz Theory, we need an analytical continuation into complex space:
- $\omega_k \in \mathbb{R} \hookrightarrow \omega_k \in \mathbb{C}$, this is SU(3) $\hookrightarrow$ SL(3,$\mathbb{C}$) and $P^\dagger \to P^{-1}$ in S.

$$\Rightarrow \quad \det(M[P]) = \det\left(2\cosh(N_\tau \sinh^{-1}(m))\mathbb{I} + e^{N_\tau \mu} P + e^{-N_\tau \mu} P^{-1}\right)$$

.

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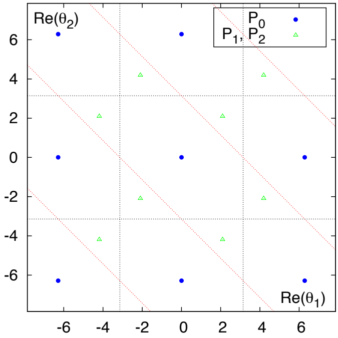
C. Schmidt and F. Ziesché, Proc. LATTICE2016, arXiv 1701.08959

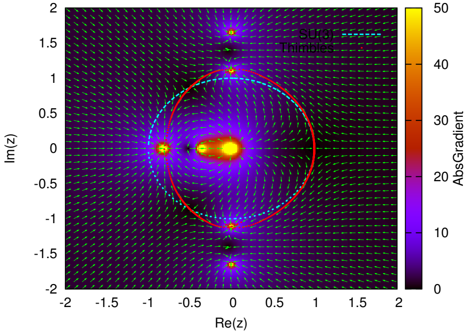
- The main critical points obtained are

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

These are the center elements of SU(3).

- The thimbles end in infinite action barriers in complexified space.





Getting the points for the triangles.

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1. Start at a saddle point.
2. Go an ϵ-step in direction of the Takagi-Vectors defined by

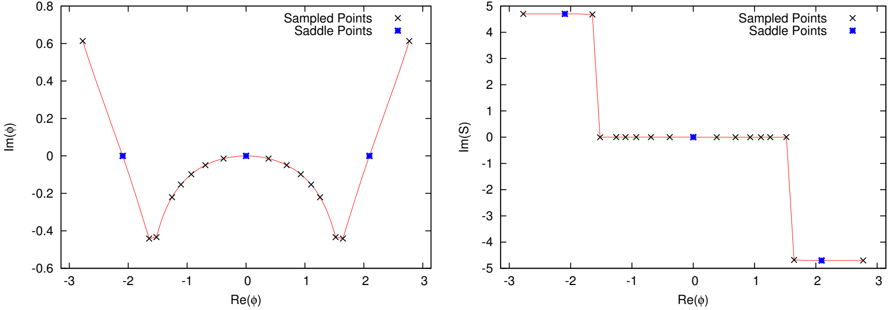
$$H(\omega_\sigma)^* \hat{\omega}_\sigma^* = \lambda \hat{\omega}_\sigma, \quad \lambda \in \mathbb{R}^+$$

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 $S \geq S_{\text{CutOff}}$ and record the points.
5. Reduce the number of points depending on a maximal discrete curvature.

Getting the points for the triangles.



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

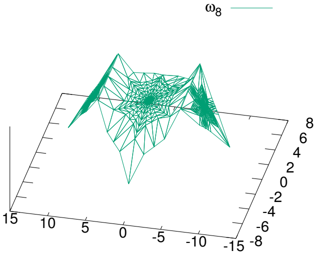
Building the triangulation

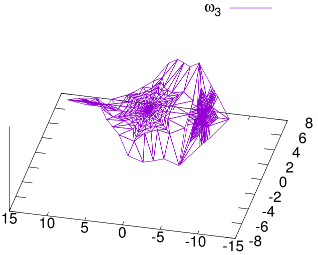
We take two neighboring flowlines consisting of the points $\{p_1^0, p_1^1, p_1^2, \dots\}$ and $\{p_2^0, p_2^1, p_2^2, \dots\}$, where $p_1^0 = p_2^0$ is the common critical point. We connect both flowlines for themselves and define $\tilde{l}_i^k := l_i^k / L_i$ to be the normalised distance to the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

Triangles $\rightarrow$ n-simplices.





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

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 rejection sampling!

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

Sampling the triangulation (RW-Slice Sampling)

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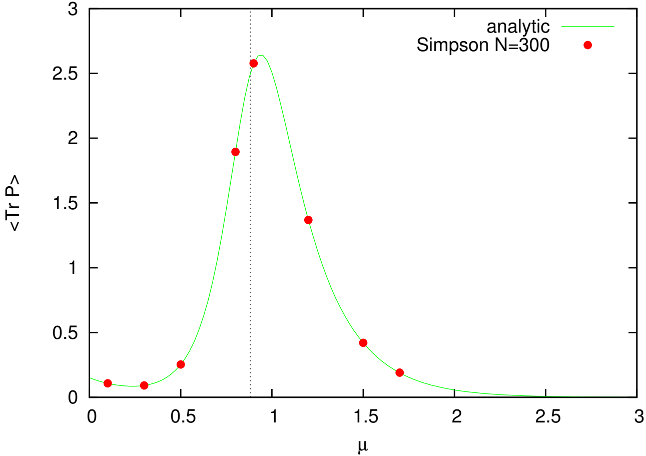
1. Select starting point P_0 on the triangulation.
2. Pick a random number $u \in [\exp(-S_{\mathrm{CutOff}}), \exp(-S_R(P_n))]$ uniformly.
3. Pick P_{n+1} from an isotropic, ergodic distrib. around P_n on the triangulation.
4. Accept P_{n+1}, if $\exp(-S_R(\tilde{P}_{n+1})) > u$. Otherwise $P_n = P_{n+1}$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

Results (at least for ω_8)



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

Lattice Gauge Theories

In full Lattice Gauge Theories new problems arise:

- We have only degenerate critical points, because of gauge symmetries.
- $\rightarrow$ Normal Picard-Lefschetz theory does not apply anymore.
- The dimensionality is quite high in general!

But we have some good news:

- We can apply the concept of Generalized Lefschetz Thimbles (*E. Witten, arXiv 1001.2933*)
- One flavor $\mathrm{U}(N_c)$ theories at finite μ have trivial GLTs, where this can be tested.
- More freedom gives us more tools than just the flow equations!

A simple U(1)-integral

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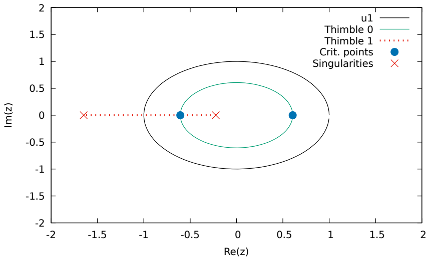
$$f(U) = 2\cosh(K_c) + e^K U + e^{-K} U^{-1}, \quad U \in \mathrm{U}(1)$$

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

- 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?

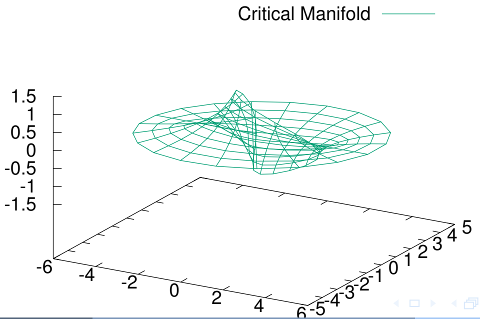
Gauge orbits

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

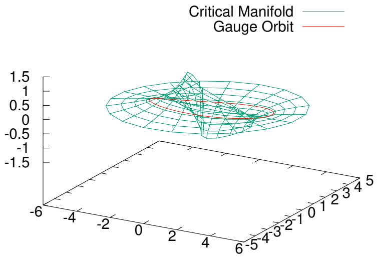
- The critical equation goes to

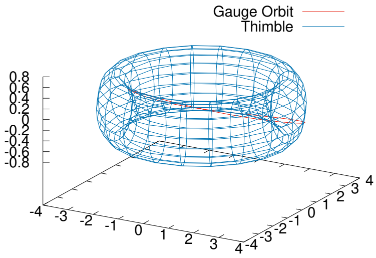
$$e^{i(\phi_1+\phi_2)} = \pm e^{-K} \Rightarrow \ \phi_1^R + \phi_2^R = 0/\pi \mod 2\pi, \ \ \phi_1^I + \phi_2^I = K$$

- So we have two 2-dimensional critical manifolds.



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.





Outlook

- We currently apply this procedure to pure gauge $\mathrm{U}(1)$-theory at $\beta \in \mathbb{C}$.
  $\rightarrow$ Results will hopefully follow soon!
- We still have to complete the sampling on triangulations and implement for higher dimensions.
- More effective Storage of the manifold by fitting the triangulation with spherical harmonics.

Thank you for your attention!

Some Important theorems

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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 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

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

... 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

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

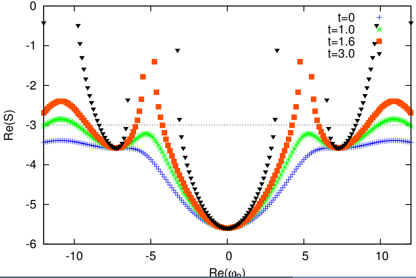
... with $H^{kl} = h_\gamma\delta^{kl}$, we have as solutions

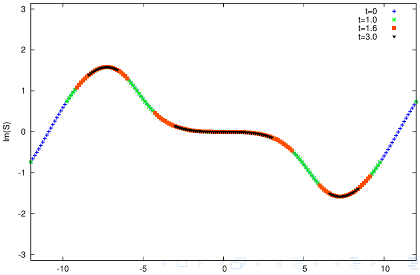
$$\lambda = |h_\gamma|, \quad \rho_\lambda^k = ce^k \quad \text{with} \quad c = \sqrt{\frac{h_\gamma^*}{|h_\gamma|}}.$$

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

- $S_I[P(t)] = \mathrm{const.}$, 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 $e^1, \dots, e^8$ along F_t by integrating $\frac{\mathrm{d}v_k}{\mathrm{d}t} = \left(\sum_{l=1}^{8} \frac{\partial^2 S}{\partial \omega_k \partial \omega_l} v_l\right)^*$, $\Rightarrow \det[\mathrm{d}F_t] = \det[v^1(t), \dots, v^8(t)]$.
5. Calculate $S_{\mathrm{eff}} = S_R - \log|\det[\mathrm{d}F_t]|$
6. Accept $\tilde{P}_{n+1}$ with probability $\min\{1, e^{-(S_{\mathrm{eff}}(\tilde{P}_{n+1}) - S_{\mathrm{eff}}(\tilde{P}_n))}\}$, otherwise $P_{n+1} = P_n$ and repeat from 2.

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

Effect of F_t on the simulation

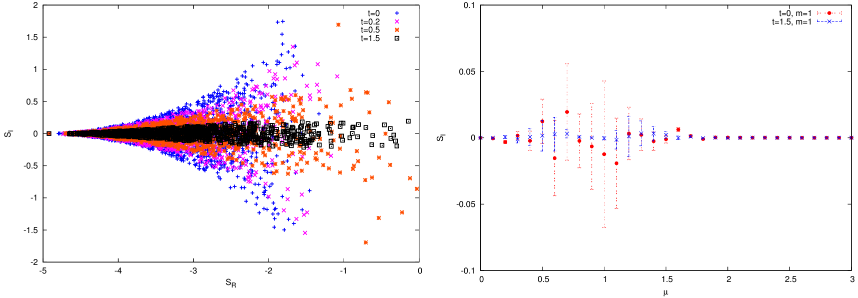


Figure: Scatterplot of sampled configurations for $m = 0.1, \mu = 0.35$ and the variations of S_I for $t = 1.5$ and $m = 1$ compared with normal Reweighting.

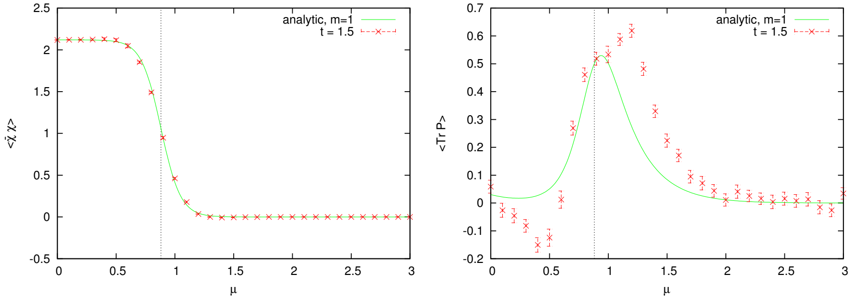
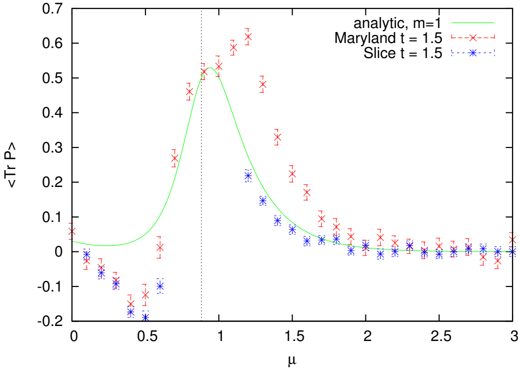


Figure: Results for $N_\tau = 4$, $m = 1.0$ using the effective action.

This is obviously wrong.

Contraction vs. Slice Sampling



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

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

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