Simulating low dimensional finite density QCD on Lefschetz Thimbles

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Motivation: The sign problem

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

$\rightarrow \quad \frac{e^{-S}}{\int_\Gamma \mathrm{d}U e^{-S}}$ is no probability density anymore.

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

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

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

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

The model: One flavor 0+1d-QCD

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

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

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

The Monodromy theorem

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

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

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

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

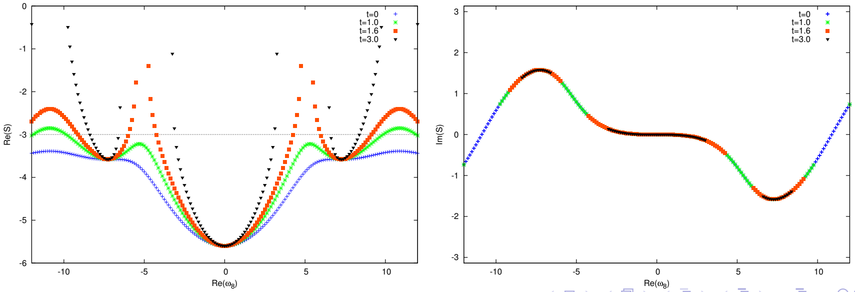
We take $\Gamma = \mathrm{SU}(3)$, whose complexification is $\tilde{\Gamma} = \mathrm{SL}(3, \mathbb{C})$.
S can be analytically continued into $\mathrm{SL}(3, \mathbb{C})$ by replacing $P^{\dagger}$ with P^{-1}.

Steepest ascent equation

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

- $S_I[P(t)] = \mathrm{const.}$, 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 $S_{\mathrm{eff}} = S_R - \log|\det[\mathrm{d}F_t]|$
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.

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

Comparison to Reweighting

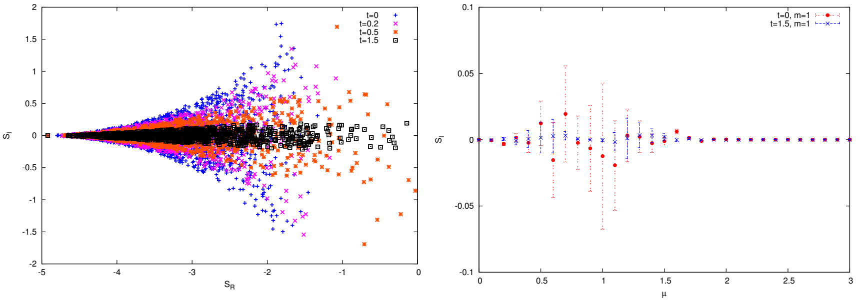
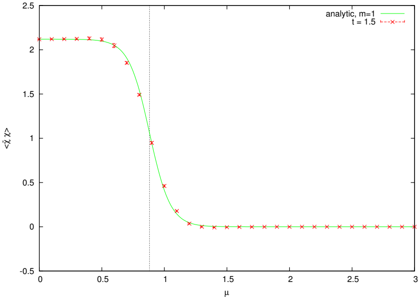


Figure: Scatterplot of sampled configurations for $m = 0.1, \mu = 0.35$ and the variations of S_I for $t = 1.5$ and $m = 1$ compared with normal Reweighting.

Results for m=1



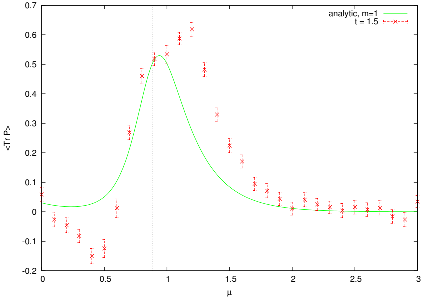


Figure: Results for $N_\tau = 4, m = 1.0$ using the effective action.

More sophisticated approach needed.

Lefschetz thimbles

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

$$Z = \int_{\mathrm{SU}(3)} \mathrm{d}P e^{-S}$$

- S has only non-degenerate crit. points: $\frac{\partial S}{\partial \omega_k}(P_\sigma) = 0 \,\forall\, k$, $\det\left[\frac{\partial^2 S}{\partial \omega_k \partial \omega_l}\right](P_\sigma) \neq 0$
- $\Rightarrow$ Lefschetz thimbles

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

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

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

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

The geometric structure of 0+1d-QCD

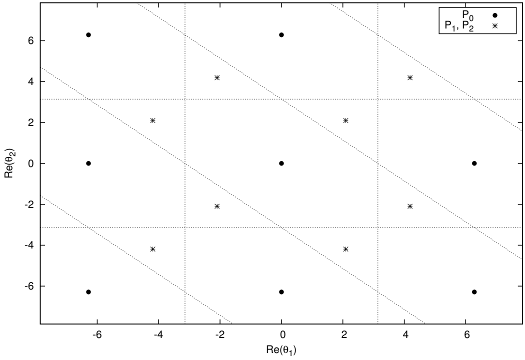
C. Schmidt and F. Ziesché, Proc. LATTICE2016, arXiv 1701.08959

- 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

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

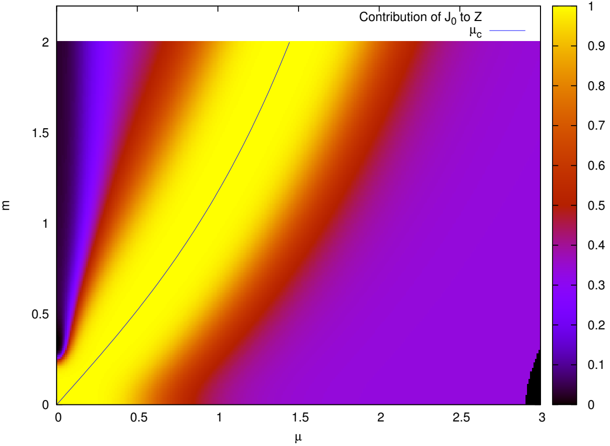
Z_σ cannot be calculated directly by Monte Carlo. But at least, we want to know how much each partition sum contributes.
$\rightarrow$ We approximate S around its critical points to get an estimate (Di Renzo, Eruzzi - Gaussian Approximation - see Lattice 2016):

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

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

Which one contributes where... an approximation

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



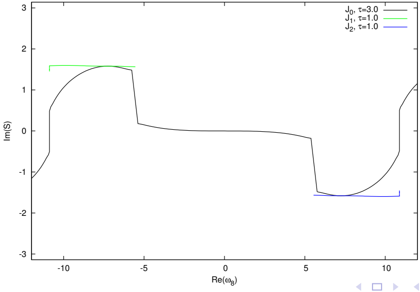
$$\frac{|Z_0|}{\sum_\sigma |Z_\sigma|}$$

Metropolis on LTs

A. Mukherjee, Phys. Rev. D88, 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 $(e^1, \ldots, e^8)$ 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_σ and proposal width d_σ have to be tuned according to the Thimble.



Outlook

- 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 Lefschetzt 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

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

... 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

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