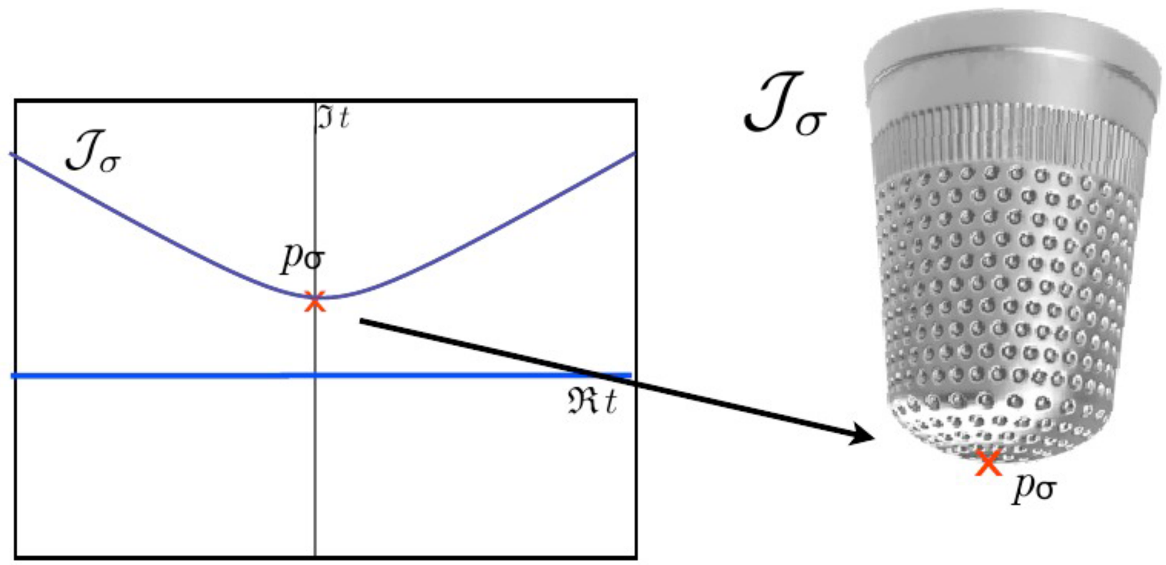
Simulating thimble regularization of lattice quantum field theories (including LGT)



Francesco Di Renzo
and G. Eruzzi

University of Parma and INFN

Lattice 2016

Southampton, 27-07-2016

Thimble regularization

(E. Witten, arXiv:1001.2933)

(M. Cristoforetti, F. Di Renzo, L. Scorzato - Phys.Rev.D88 2013 and Y. Kikukawa et al JHEP 1310)

has still a long way to go. In particular, Monte Carlo simulations on thimbles are a non-trivial task. Also, gauge theories are tricky (but they are in the end a final goal we do not want to really live without).

In the context of the chiral random matrix model we introduced an approach to computations on thimbles which takes into account the contributions from complete flow lines: can it be turned into a Monte Carlo? Is it any useful for SU(N)?

In the context of the Bose gas, what we call the gaussian approximation worked pretty well (maybe even better than one could hope/expect): what about its applicability to gauge theories?

Agenda

- Complete flow lines as basic degrees of freedom and a Monte Carlo algorithm for such an approach.

- Basic formalism for SU(N)

- Some (basic…) steps into gauge theories: QCD in 0+1 dimensions

- Basics on the real thing: thimbles and the gauge structure of SU(N)

- Gaussian approximation for SU(N) (N=2 in d=2, actually)

When you have a complex action in place (sign problem) …

… it can be a good idea to compute observables in thimble regularization

$$\langle O \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n z \, O(z) e^{-S_R(z)} = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, O \, e^{-S_R} \, e^{i\,\omega}$$

$$Z = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n z \, e^{-S_R(z)} = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, e^{-S_R} \, e^{i\,\omega}$$

$$\mathcal{J}_\sigma \equiv \left\{ z(0) \in \mathcal{X} \,\middle|\, \dot{z}^i = g^{i\bar{j}} \partial_{\bar{j}} \bar{S}, \lim_{t \to -\infty} z(t) = z_\sigma \right\} \subset \mathcal{X}$$

Thimbles are manifolds which live in the complexification of the original manifold your theory is defined on. They are the union of the Steepest Ascent paths attached to critical points, on which the imaginary part of the action stays constant. Their real dimension is just the same as that of the original manifold.

When you have a complex action in place (sign problem) …

… it can be a good idea to compute observables in thimble regularization

$$\langle O \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n z \, O(z) e^{-S_R(z)} = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, O \, e^{-S_R} \, e^{i\,\omega}$$

$$Z = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n z \, e^{-S_R(z)} = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, e^{-S_R} \, e^{i\,\omega}$$

$$\mathcal{J}_\sigma \equiv \left\{ z(0) \in \mathcal{X} \,\middle|\, \dot{z}^i = g^{i\bar{j}} \partial_{\bar{j}} \bar{S}, \lim_{t \to -\infty} z(t) = z_\sigma \right\} \subset \mathcal{X}$$

Thimbles are manifolds which live in the complexification of the original manifold your theory is defined on. They are the union of the Steepest Ascent paths attached to critical points, on which the imaginary part of the action stays constant. Their real dimension is just the same as that of the original manifold.

The tangent space at the critical point is spanned by the Takagi vectors of the Hessian

$$H(S; p_\sigma) v^{(i)} = \lambda_i \bar{v}^{(i)}$$

In general at each point an orthonormal basis of the tangent space induces the natural coordinate system …

$$\varphi\left(z + \sum_{i=1}^{n} \delta y_i \, U^{(i)} \right) = \delta y + \mathcal{O}\left(\delta y^2\right) \in \mathbb{R}^n \qquad \int_{\Gamma_z} \mathrm{d}^n z \, f(z) = \int_{\varphi(\Gamma_z)} \mathrm{d}^n \delta y \, f\left(\varphi^{-1}\left(\delta y\right)\right) \det U \left(\varphi^{-1}\left(\delta y\right)\right) \qquad \delta z = \sum_i \delta y_i \, U^{(i)}$$

… but we only know a basis for the tangent space if we transport the vector basis that we know at the critical point

$$\frac{\mathrm{d}V_j}{\mathrm{d}t} = \sum_{i=1}^{n} \bar{V}_i \overline{\left(\frac{\partial^2 S}{\partial z^i \partial z^j} \right)}$$

Complete flow lines formalism
and a Monte Carlo algorithm for such an approach

A natural way to rephrase integrals on thimbles

$$\langle O \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-i S_I(z_\sigma)} Z_\sigma \, \langle\langle O \, e^{i\,\omega} \rangle\rangle_\sigma \qquad \langle\langle \bullet \rangle\rangle_\sigma \equiv \frac{1}{Z_\sigma} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, \bullet \, e^{-S_R}$$

with the partition function given by $$Z = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-i S_I(z_\sigma)} Z_\sigma \, \langle\langle e^{i\,\omega} \rangle\rangle_\sigma$$

A natural way to rephrase integrals on thimbles

$$\langle O \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} Z_\sigma \, \langle\langle O \, e^{i\,\omega} \rangle\rangle_\sigma \qquad \langle\langle \bullet \rangle\rangle_\sigma \equiv \frac{1}{Z_\sigma} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, \bullet \, e^{-S_R}$$

with the partition function given by $\quad Z = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} Z_\sigma \, \langle\langle e^{i\,\omega} \rangle\rangle_\sigma$

For the sake of simplicity we now specify to the case of only one thimble in place. Now expectation values are restricted to that thimble (we drop double wedges and footer)

$$\langle O \rangle \rightarrow \frac{\langle O \, e^{i\,\omega} \rangle}{\langle e^{i\,\omega} \rangle} \qquad \langle \bullet \rangle = \frac{\int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, \bullet \, e^{-S_R}}{\int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, e^{-S_R}}$$

A natural way to rephrase integrals on thimbles

$$\langle O \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} Z_\sigma \, \langle\langle O \, e^{i\,\omega} \rangle\rangle_\sigma \qquad \langle\langle \bullet \rangle\rangle_\sigma \equiv \frac{1}{Z_\sigma} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, \bullet \, e^{-S_R}$$

with the partition function given by $Z = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} Z_\sigma \, \langle\langle e^{i\,\omega} \rangle\rangle_\sigma$

For the sake of simplicity we now specify to the case of only one thimble in place. Now expectation values are restricted to that thimble (we drop double wedges and footer)

$$\langle O \rangle \rightarrow \frac{\langle O \, e^{i\,\omega} \rangle}{\langle e^{i\,\omega} \rangle} \qquad \langle \bullet \rangle = \frac{\int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, \bullet \, e^{-S_R}}{\int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, e^{-S_R}}$$

A very natural parametrization of the thimble (see also Kikukawa et al JHEP1310)

$$\mathcal{J}_\sigma \ni z \leftrightarrow (\hat{n}, t) \in S^{n-1}_{\mathcal{R}} \times \mathbb{R}$$

whose meaning is easy to understand: each point on a SA (flow line) is identified by the direction (on the tangent space) you take when you leave the critical point (this singles out the flow line itself) and the flow time at which you reach the point.

In practice: you make a choice for a direction on the tangent space $\sum_{i=1}^{n} n_i v^{(i)}$ with $\sum_{i=1}^{n} n_i^2 = \mathcal{R}$

Near the critical point natural coordinates are given in terms of the basis provided by the Takagi vectors of H. Then the action is $S(\eta) = S(z_\sigma) + \frac{1}{2}\sum_{i=1}^{n} \lambda_i \eta_i^2$

and the evolution along a flow line is given by $\eta_i(t) = n_i\, e^{\lambda_i t}$

and $V^{(i)}(t) = v^{(i)}\, e^{\lambda_i t}$

i.e. $z_j(t) = \; z_\sigma + \sum_{k=1}^{n} n_k\, e^{\lambda_k t}\, v_j^{(k)}$

which at a convenient value of (remote) time is our initial condition for the SA.

In practice: you make a choice for a direction on the tangent space $\sum_{i=1}^{n} n_i v^{(i)}$ with $\sum_{i=1}^{n} n_i^2 = \mathcal{R}$

Near the critical point natural coordinates are given in term of the basis provided by the Takagi vectors. Then the action is $S(\eta) = S(z_\sigma) + \frac{1}{2}\sum_{i=1}^{n} \lambda_i \eta_i^2$

and the evolution along a flow line is given by $\eta_i(t) = n_i\, e^{\lambda_i t}$

and $V^{(i)}(t) = v^{(i)}\, e^{\lambda_i t}$

i.e. $z_j(t) = z_\sigma + \sum_{k=1}^{n} n_k\, e^{\lambda_k t}\, v_j^{(k)}$

which at a convenient value of (remote) time is our initial condition for the SA.

Now we want to express the integral on the thimble as an
integral over directions and flow times

In practice: you make a choice for a direction on the tangent space $\sum_{i=1}^{n} n_i v^{(i)}$ with $\sum_{i=1}^{n} n_i^2 = \mathcal{R}$

Near the critical point natural coordinates are given in term of the basis provided by the Takagi vectors. Then the action is $S(\eta) = S(z_\sigma) + \frac{1}{2}\sum_{i=1}^{n} \lambda_i \eta_i^2$

and the evolution along a flow line is given by $\eta_i(t) = n_i\, e^{\lambda_i t}$

and $V^{(i)}(t) = v^{(i)}\, e^{\lambda_i t}$

i.e. $z_j(t) = z_\sigma + \sum_{k=1}^{n} n_k\, e^{\lambda_k t}\, v_j^{(k)}$

which at a convenient value of (remote) time is our initial condition for the SA.

Now we want to express the integral on the thimble as an
integral over directions and flow times

Basically we play a Faddeev-Popov trick … $1 = \Delta_{\hat{n}}(t) \int \prod_{k=1}^{n} \mathrm{d}n_k\, \delta\left(|\vec{n}|^2 - \mathcal{R}\right) \int \mathrm{d}t \prod_{i=1}^{n} \delta\left(\delta y_i - \delta y_i(\hat{n}, t)\right)$

$$1 = \Delta_{\hat{n}}(t) \int \prod_{k=1}^{n} \mathrm{d}n'_k\, \delta\left(|\vec{n}'|^2 - \mathcal{R}\right) \int \mathrm{d}t' \prod_{i=1}^{n} \delta\left(\delta y_i - \delta y_i(\hat{n}', t')\right)$$

$$= \Delta_{\hat{n}}(t) \int \prod_{k=1}^{n} \mathrm{d}n'_i \prod_{i=1}^{n} \delta\left(n'_i - n_i\right) \int \mathrm{d}t'\, \delta\left(t' - t\right) \left| \frac{\partial\left(|\vec{n}'|^2 - \mathcal{R}, \delta y_i - \delta y_i(\hat{n}', t')\right)}{\partial\left(t', \hat{n}'\right)} \right|^{-1}$$

$$= \Delta_{\hat{n}}(t) \left| \frac{\partial\left(|\vec{n}|^2 - \mathcal{R}, \delta y_i - \delta y_i(\hat{n}, t)\right)}{\partial\left(t, \hat{n}\right)} \right|^{-1}$$

All in all

$$Z = \int \mathcal{D}\hat{n}\, Z_{\hat{n}} \qquad \mathcal{D}\hat{n} \equiv \prod_{k=1}^{n} \mathrm{d}n_k \delta\left(|\vec{n}|^2 - \mathcal{R}\right) \qquad Z_{\hat{n}} = \int_{-\infty}^{+\infty} \mathrm{d}t\, \Delta_{\hat{n}}(t)\, e^{-S_R(\hat{n},t)}$$

and it turns out that

$$Z_{\hat{n}} = 2\sum_{i=1}^{n} \lambda_i n_i^2 \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-S_{\mathrm{eff}}(\hat{n},t)} \qquad S_{\mathrm{eff}}(\hat{n},t) = S_R(\hat{n},t) - \log|\det V(t)|$$

All in all

$$Z = \int \mathcal{D}\hat{n}\, Z_{\hat{n}} \qquad \mathcal{D}\hat{n} \equiv \prod_{k=1}^{n} \mathrm{d}n_k \delta\left(|\vec{n}|^2 - \mathcal{R}\right) \qquad Z_{\hat{n}} = \int_{-\infty}^{+\infty} \mathrm{d}t\, \Delta_{\hat{n}}(t)\, e^{-S_R(\hat{n},t)}$$

and it turns out that

$$Z_{\hat{n}} = 2\sum_{i=1}^{n} \lambda_i n_i^2 \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-S_{\mathrm{eff}}(\hat{n},t)} \qquad S_{\mathrm{eff}}(\hat{n},t) = S_R(\hat{n},t) - \log|\det V(t)|$$

Defining $\langle A \rangle_{\hat{n}} = \dfrac{\int_{-\infty}^{+\infty} dt \Delta_{\hat{n}}(t) e^{-S_R(\hat{n},t)} A}{Z_{\hat{n}}}$

we have in the end

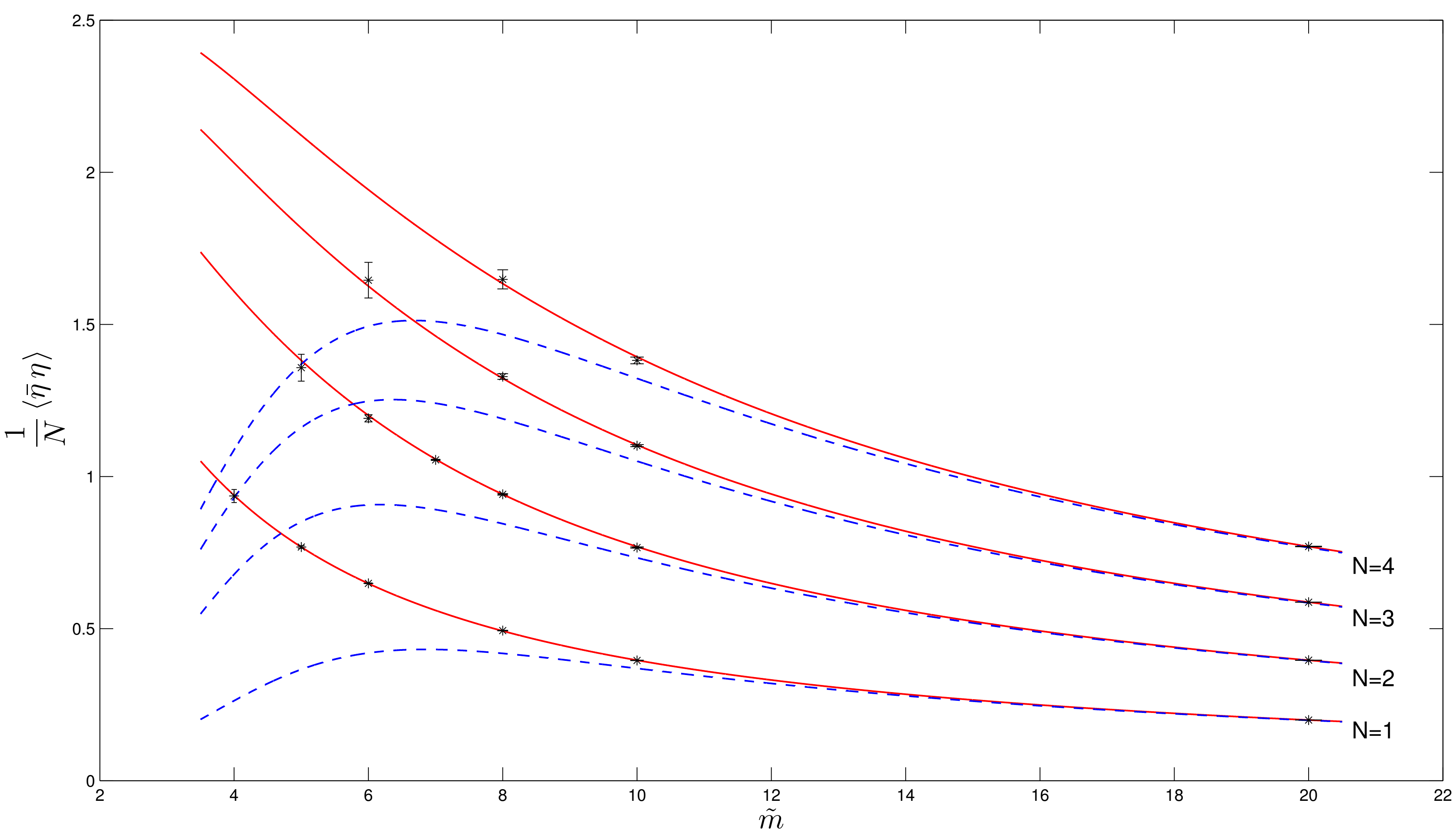
$$\langle O \rangle = \frac{\int \mathcal{D}\hat{n}\, Z_{\hat{n}} \left\langle e^{i\omega} O \right\rangle_{\hat{n}}}{\int \mathcal{D}\hat{n}\, Z_{\hat{n}} \left\langle e^{i\omega} \right\rangle_{\hat{n}}}$$

GOOD! This is a new average, again with a positive measure. Once we prepare an initial condition we go all the way up the flow line (problem of staying on the thimble solved)

$$\langle O \rangle = \frac{\int \mathcal{D}\hat{n}\; Z_{\hat{n}} \left\langle e^{i\omega} O \right\rangle_{\hat{n}}}{\int \mathcal{D}\hat{n}\; Z_{\hat{n}} \left\langle e^{i\omega} \right\rangle_{\hat{n}}}$$

PROBLEM! Difficult to sample by Monte Carlo, so at first we went through the very basic one: flat, crude Monte Carlo …

… which nevertheless worked for the Chiral Random Matrix Model (Di Renzo, Eruzzi PhysRev D92)



A new Monte Carlo

First of all: for a gaussian thimble (one for which $S(\eta) = S(z_\sigma) + \frac{1}{2}\sum_{i=1}^{n} \lambda_i \eta_i^2$ holds everywhere)

$$Z_{\hat{n}} = 2 \sum_i n_i^2 \lambda_i \int_{-\infty}^{+\infty} dt \; e^{\Lambda t - \frac{1}{2}\sum_i n_i^2 \lambda_i e^{2\lambda_i t}} \qquad \Lambda = \sum_i \lambda_i$$

This we can sample by heat bath with a method we all teach our students

$$F(x) = P(X < x) = \int_{-\infty}^{x} f(y) dy \qquad \xi \in [\,0, 1\,] \;\; \text{flat random} \qquad F^{-1}(\xi)$$

A new Monte Carlo

First of all: for a gaussian thimble (one for which $S(\eta) = S(z_\sigma) + \frac{1}{2}\sum_{i=1}^{n} \lambda_i \eta_i^2$ holds everywhere)

$$Z_{\hat{n}} = 2\sum_i n_i^2 \lambda_i \int_{-\infty}^{+\infty} dt\; e^{\Lambda t - \frac{1}{2}\sum_i n_i^2 \lambda_i e^{2\lambda_i t}} \qquad \Lambda = \sum_i \lambda_i$$

This we can sample by heat bath with a method we all teach our students

$$F(x) = P(X < x) = \int_{-\infty}^{x} f(y)dy \qquad \xi \in [0,1] \;\; \text{flat random} \qquad F^{-1}(\xi)$$

Simply pick a couple $\quad n_i^2 + n_j^2 = R - \sum_{k\neq i,j} n_k^2 = C \qquad n_i = \sqrt{C}cos(\phi)\;,\; n_j = \sqrt{C}sin(\phi)$

and notice that $\quad Z_{\hat{n},i,j}(\phi) = 2\left[\sum_{k\neq i,j} n_k^2\lambda_k + \lambda_i C cos^2(\phi) + \lambda_j C sin^2(\phi)\right]\int_{-\infty}^{+\infty} dt\; e^{\Lambda t - S(\phi,t)}$

with $\quad S(\phi,t) = \frac{1}{2}\left[\sum_{k\neq i,j} n_k^2\lambda_k e^{2\lambda_k t} + Ccos^2(\phi) n_i^2 \lambda_i e^{2\lambda_i t} + Csin^2(\phi) n_j^2 \lambda_j e^{2\lambda_j t}\right]$

defines a probability $\quad P_{\hat{n},i,j}(\phi) = \dfrac{Z_{\hat{n},i,j}(\phi)}{\int_0^{2\pi} d\psi Z_{\hat{n},i,j}(\psi)}$

for which we can play the above trick: this is a HEAT BATH for the gaussian thimble

A new Monte Carlo

1. You sit on a $\hat{n}$
2. Extract (by gaussian heat bath) a new $\hat{n}'$ (connected by the rotation we saw)
3. Perform the SA defined by $\hat{n}'$ and compute $Z_{\hat{n}'}$
4. Accept with probability

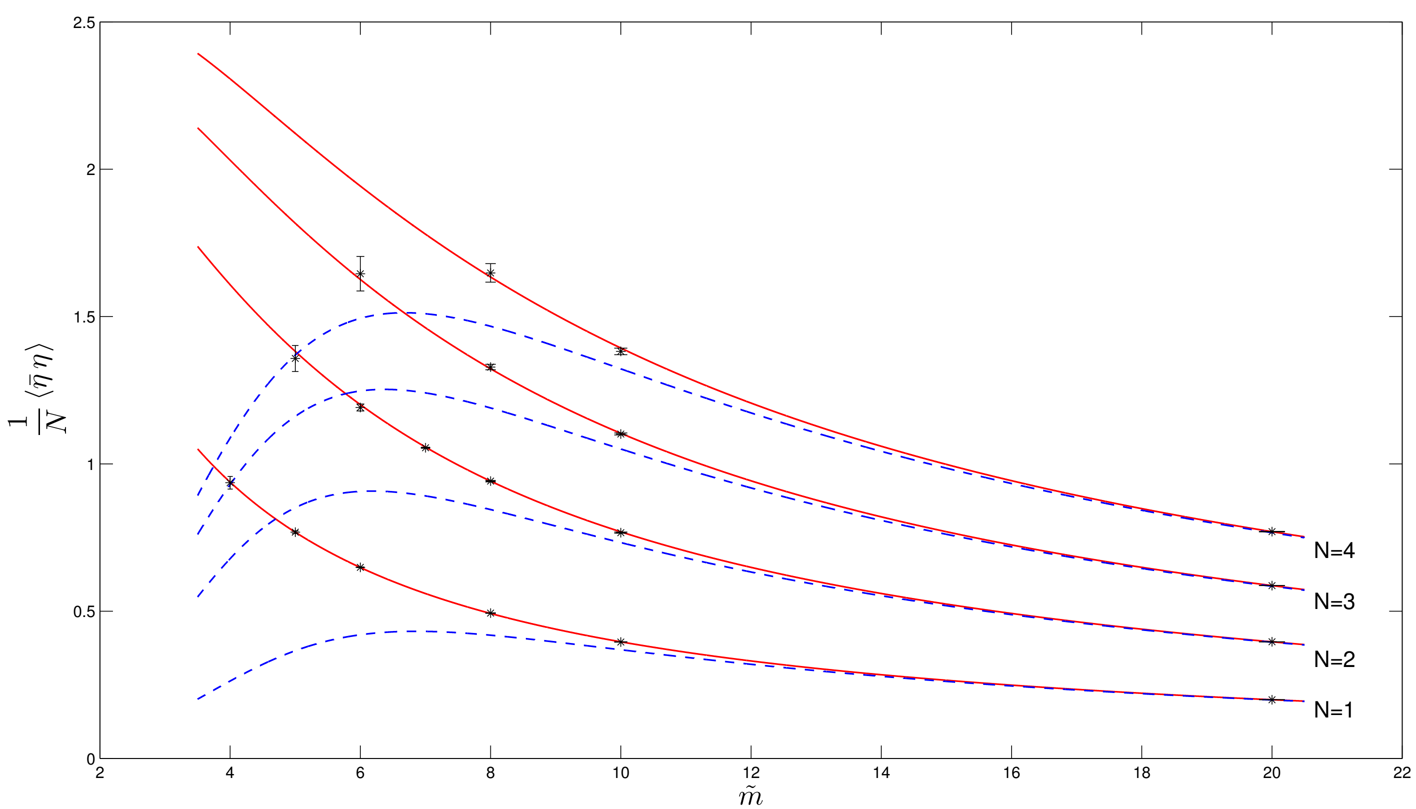
$$\min\left\{\frac{Z^{(G)}_{\hat{n}}}{Z^{(G)}_{\hat{n}'}}\,\frac{Z_{\hat{n}'}}{Z_{\hat{n}}}\right\}$$

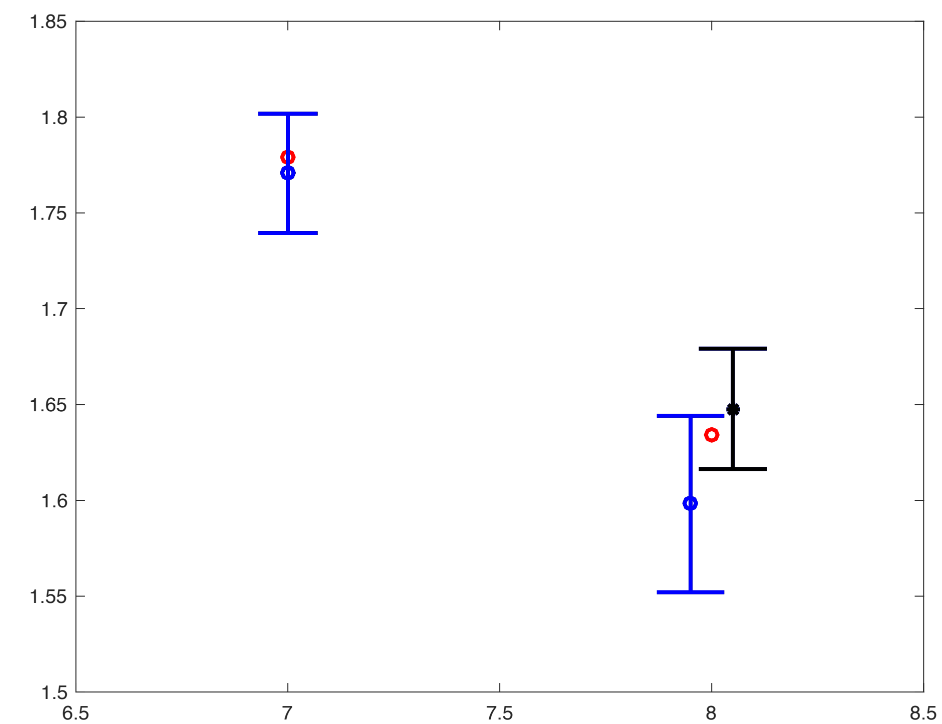
A new Monte Carlo

1. You sit on a $\hat{n}$
2. Extract (by gaussian heat bath) a new $\hat{n}'$ (connected by the rotation we saw)
3. Perform the SA defined by $\hat{n}'$ and compute $Z_{\hat{n}'}$
4. Accept with probability

$$\min\left\{ \frac{Z^{(G)}_{\hat{n}}}{Z^{(G)}_{\hat{n}'}} \frac{Z_{\hat{n}'}}{Z_{\hat{n}}} \right\}$$

It works! Again CRMM …





RED exact BLUE new (1.3K samples at m=8)
BLACK old (122K samples at m=8!)

Basic formalism for SU(N)

The relevant basic set-up we need

Going to complex fields means $\mathrm{SU}(N) \ni U = e^{ix_a T^a} \to e^{iz_a T^a} = e^{i(x_a + iy_a)T^a} \in \mathrm{SL}(N, \mathbb{C})$

In $\mathrm{SL}(N, \mathbb{C})$, $U^\dagger \neq U^{-1}$ i.e. $\mathrm{SU}(N) \ni U^\dagger = e^{-ix_a T^a} \to e^{-iz_a T^a} = e^{-i(x_a + iy_a)T^a} = U^{-1} \in \mathrm{SL}(N, \mathbb{C})$

Main ingredient is the Lie derivative

$$\nabla^a f(U) = \lim_{\alpha \to 0} \frac{1}{\alpha} \left[f\left(e^{i\alpha T^a} U\right) - f(U) \right] = \frac{\partial}{\partial \alpha} f\left(e^{i\alpha T^a} U\right) \Big|_{\alpha=0}$$

Namely

$$\begin{aligned}
\nabla^a f(U) &:= \frac{\partial}{\partial \alpha} f\left(e^{i\alpha T^a} U\right) \Big|_{\alpha=0} \\
\nabla^a f\left(U^\dagger\right) &:= 0 \\
\bar{\nabla}^a f\left(U^\dagger\right) &:= \frac{\partial}{\partial \alpha} f\left(U^\dagger e^{-i\alpha T^a}\right) \Big|_{\alpha=0} \\
\bar{\nabla}^a f(U) &:= 0
\end{aligned}$$

and the SA (SD) equations are

$$\frac{d}{dt} z(t) = \frac{\partial \bar{S}[\bar{z}]}{\partial \bar{z}} \quad \rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}\tau} U_{\hat{\mu}}(n;\tau) = \left(i\, T^a \bar{\nabla}^a_{n,\hat{\mu}} \overline{S\left[U(\tau)\right]} \right) U_{\hat{\mu}}(n;\tau)$$

Be careful with

$$
\begin{aligned}
\left[\nabla^a_{n,\hat{\mu}}\,,\nabla^b_{m,\hat{\nu}}\right] &= -f^{abc}\,\nabla^c_{n,\hat{\mu}}\,\delta_{n,m}\delta_{\hat{\mu},\hat{\nu}} \\
\left[\bar{\nabla}^a_{n,\hat{\mu}}\,,\bar{\nabla}^b_{m,\hat{\nu}}\right] &= -f^{abc}\,\bar{\nabla}^c_{n,\hat{\mu}}\,\delta_{n,m}\delta_{\hat{\mu},\hat{\nu}} \\
\left[\nabla^a_{n,\hat{\mu}}\,,\bar{\nabla}^b_{m,\hat{\nu}}\right] &= 0
\end{aligned}
$$

Be careful with

$$\begin{aligned} \left[\nabla^a_{n,\hat\mu}\,,\nabla^b_{m,\hat\nu}\right] &= -f^{abc}\,\nabla^c_{n,\hat\mu}\,\delta_{n,m}\delta_{\hat\mu,\hat\nu} \\ \left[\bar\nabla^a_{n,\hat\mu}\,,\bar\nabla^b_{m,\hat\nu}\right] &= -f^{abc}\,\bar\nabla^c_{n,\hat\mu}\,\delta_{n,m}\delta_{\hat\mu,\hat\nu} \\ \left[\nabla^a_{n,\hat\mu}\,,\bar\nabla^b_{m,\hat\nu}\right] &= 0 \end{aligned}$$

but then all the other stuff goes through smoothly, i.e. $\frac{\mathrm{d}}{\mathrm{d}\tau} = \bar\nabla^a_{n,\hat\mu}\bar S\,\nabla^a_{n,\hat\mu} + \nabla^a_{n,\hat\mu}S\,\bar\nabla^a_{n,\hat\mu}$

$$\frac{\mathrm{d}S^R}{\mathrm{d}\tau} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(S+\bar S\right) = \frac{1}{2}\left(\bar\nabla^a_{n,\hat\mu}\bar S\,\nabla^a_{n,\hat\mu}S + \nabla^a_{n,\hat\mu}S\,\bar\nabla^a_{n,\hat\mu}\bar S\right) = \|\nabla S\|^2 \geq 0$$

along the flow

$$\frac{\mathrm{d}S^I}{\mathrm{d}\tau} = \frac{1}{2i}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(S-\bar S\right) = \frac{1}{2i}\left(\bar\nabla^a_{n,\hat\mu}\bar S\,\nabla^a_{n,\hat\mu}S - \nabla^a_{n,\hat\mu}S\,\bar\nabla^a_{n,\hat\mu}\bar S\right) = 0$$

Be careful with
$$
\begin{aligned}
\left[\nabla^a_{n,\hat{\mu}}\,,\nabla^b_{m,\hat{\nu}}\right] &= -f^{abc}\,\nabla^c_{n,\hat{\mu}}\,\delta_{n,m}\delta_{\hat{\mu},\hat{\nu}}\\
\left[\bar{\nabla}^a_{n,\hat{\mu}}\,,\bar{\nabla}^b_{m,\hat{\nu}}\right] &= -f^{abc}\,\bar{\nabla}^c_{n,\hat{\mu}}\,\delta_{n,m}\delta_{\hat{\mu},\hat{\nu}}\\
\left[\nabla^a_{n,\hat{\mu}}\,,\bar{\nabla}^b_{m,\hat{\nu}}\right] &= 0
\end{aligned}
$$

but then all the other stuff goes through smoothly, i.e. $\frac{\mathrm{d}}{\mathrm{d}\tau} = \bar{\nabla}^a_{n,\hat{\mu}}\bar{S}\,\nabla^a_{n,\hat{\mu}} + \nabla^a_{n,\hat{\mu}}S\,\bar{\nabla}^a_{n,\hat{\mu}}$

$$
\frac{\mathrm{d}S^R}{\mathrm{d}\tau} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(S+\bar{S}\right) = \frac{1}{2}\left(\bar{\nabla}^a_{n,\hat{\mu}}\bar{S}\,\nabla^a_{n,\hat{\mu}}S + \nabla^a_{n,\hat{\mu}}S\,\bar{\nabla}^a_{n,\hat{\mu}}\bar{S}\right) = \left\|\nabla S\right\|^2 \geq 0
$$

along the flow

$$
\frac{\mathrm{d}S^I}{\mathrm{d}\tau} = \frac{1}{2i}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(S-\bar{S}\right) = \frac{1}{2i}\left(\bar{\nabla}^a_{n,\hat{\mu}}\bar{S}\,\nabla^a_{n,\hat{\mu}}S - \nabla^a_{n,\hat{\mu}}S\,\bar{\nabla}^a_{n,\hat{\mu}}\bar{S}\right) = 0
$$

and as for transporting the basis

$$
V \equiv V_{n,\hat{\mu},a}\nabla^a_{n,\hat{\mu}} + \bar{V}_{n,\hat{\mu},a}\bar{\nabla}^a_{n,\hat{\mu}} \qquad\qquad \left[V,V'\right]_{n,\hat{\mu},c} = -f^{abc}\,V_{n,\hat{\mu},a}V'_{n,\hat{\mu},b}
$$

$$
V' = \bar{\nabla}\bar{S} \qquad
\begin{aligned}
\left[V,V'\right]_{n,\hat{\mu},c} &= \left(V_{m,\hat{\nu},a}\nabla^a_{m,\hat{\nu}} + \bar{V}_{m,\hat{\nu},a}\bar{\nabla}^a_{m,\hat{\nu}}\right)\bar{\nabla}^c_{n,\hat{\mu}}\bar{S} - \\
&\quad - \left(\bar{\nabla}^a_{m,\hat{\nu}}\bar{S}\,\nabla^a_{m,\hat{\nu}} + \nabla^a_{m,\hat{\nu}}S\,\bar{\nabla}^a_{m,\hat{\nu}}\right)V_{n,\hat{\mu},c} = \\
&= V_{m,\hat{\nu},a}\nabla^a_{m,\hat{\nu}}\bar{\nabla}^c_{n,\hat{\mu}}\bar{S} + \bar{V}_{m,\hat{\nu},a}\bar{\nabla}^a_{m,\hat{\nu}}\bar{\nabla}^c_{n,\hat{\mu}}\bar{S} - \frac{\mathrm{d}V_{n,\hat{\mu},c}}{\mathrm{d}\tau} = \\
&= -f^{abc}\,V_{n,\hat{\mu},a}\bar{\nabla}^b_{n,\hat{\mu}}\bar{S}
\end{aligned}
$$

$$
\frac{\mathrm{d}}{\mathrm{d}\tau}V_{n,\hat{\mu},c} = \bar{\nabla}^a_{m,\hat{\nu}}\bar{\nabla}^c_{n,\hat{\mu}}\bar{S}\,\bar{V}_{m,\hat{\nu},a} + f^{abc}\,\bar{\nabla}^b_{n,\hat{\mu}}\bar{S}\,V_{n,\hat{\mu},a}
$$

from which we can have the basis for the tangent space at any point

Some (basic…) steps into gauge theories: QCD in 0+1 dimensions

QCD in 0+1 dim

$$\mathcal{Z}_{N_f} = \int \prod_{i=1}^{N_t} \mathrm{d}U_i \, \det{}^{N_f} D \qquad (aD)_{ii'} = am\delta_{ii'} + \frac{1}{2}\left(e^{a\mu}U_i\tilde{\delta}_{i',i+1} - e^{-a\mu}U_{i-1}^\dagger\tilde{\delta}_{i',i-1}\right)$$

$$aD = \begin{pmatrix} am & e^{a\mu}U_1/2 & 0 & \cdots & 0 & e^{-a\mu}U_{N_t}^\dagger/2 \\ -e^{-a\mu}U_1^\dagger/2 & am & e^{a\mu}U_2/2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & am & e^{a\mu}U_{N_t-1}/2 \\ -e^{a\mu}U_{N_t}/2 & 0 & 0 & \cdots & -e^{-a\mu}U_{N_t-1}^\dagger/2 & am \end{pmatrix}$$

Actually in a good gauge $$\mathcal{Z}_{N_f} = \int_{\mathrm{SU}(3)} \mathrm{d}U \, \det{}^{N_f}\left(A\mathbb{1}_{3\times 3} + e^{\mu/T}U + e^{-\mu/T}U^\dagger\right)$$

We compute (anti)Polyakov loop and the chiral condensate $\Sigma = T\dfrac{\partial}{\partial m}\log\mathcal{Z}$

We have 3 critical points (Z_3 roots) and we know both the results and their semiclassical approximations

semiclassical approximation

$$Z \approx (2\pi)^4 \sum_\sigma \mathfrak{n}_\sigma \, e^{-S(U_\sigma)} \, \lambda_\sigma^{-4} \, e^{i\,\omega_\sigma} \qquad e^{i\,\omega_\sigma} = e^{-4i\,\varphi_\sigma}$$

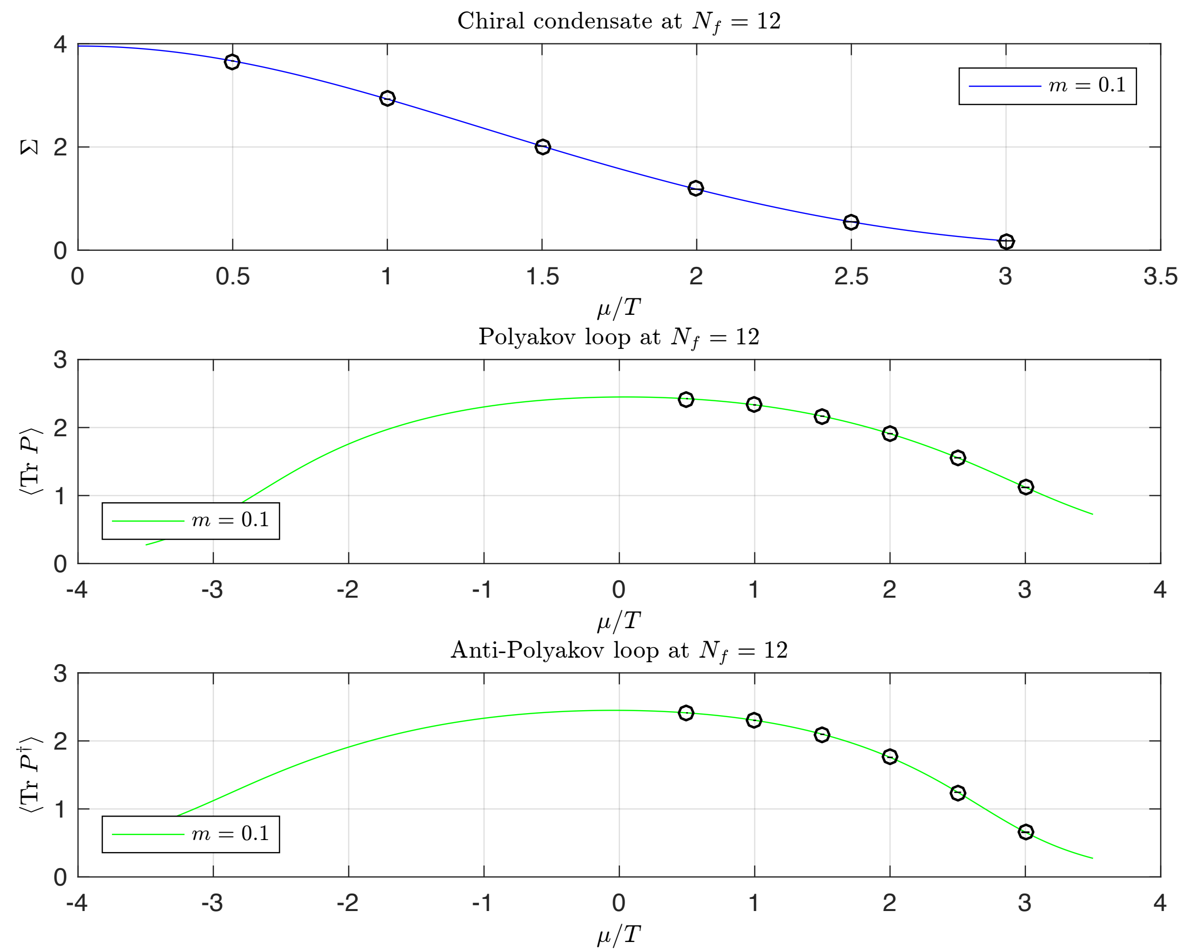
$$S(U_\sigma) = -3N_f \log B_\sigma$$

$$B_\sigma = 2\left[\cosh\left(\frac{\mu_c}{T}\right) + \cosh\left(\frac{\mu}{T} + \frac{2\pi i\, k_\sigma}{3}\right)\right]$$

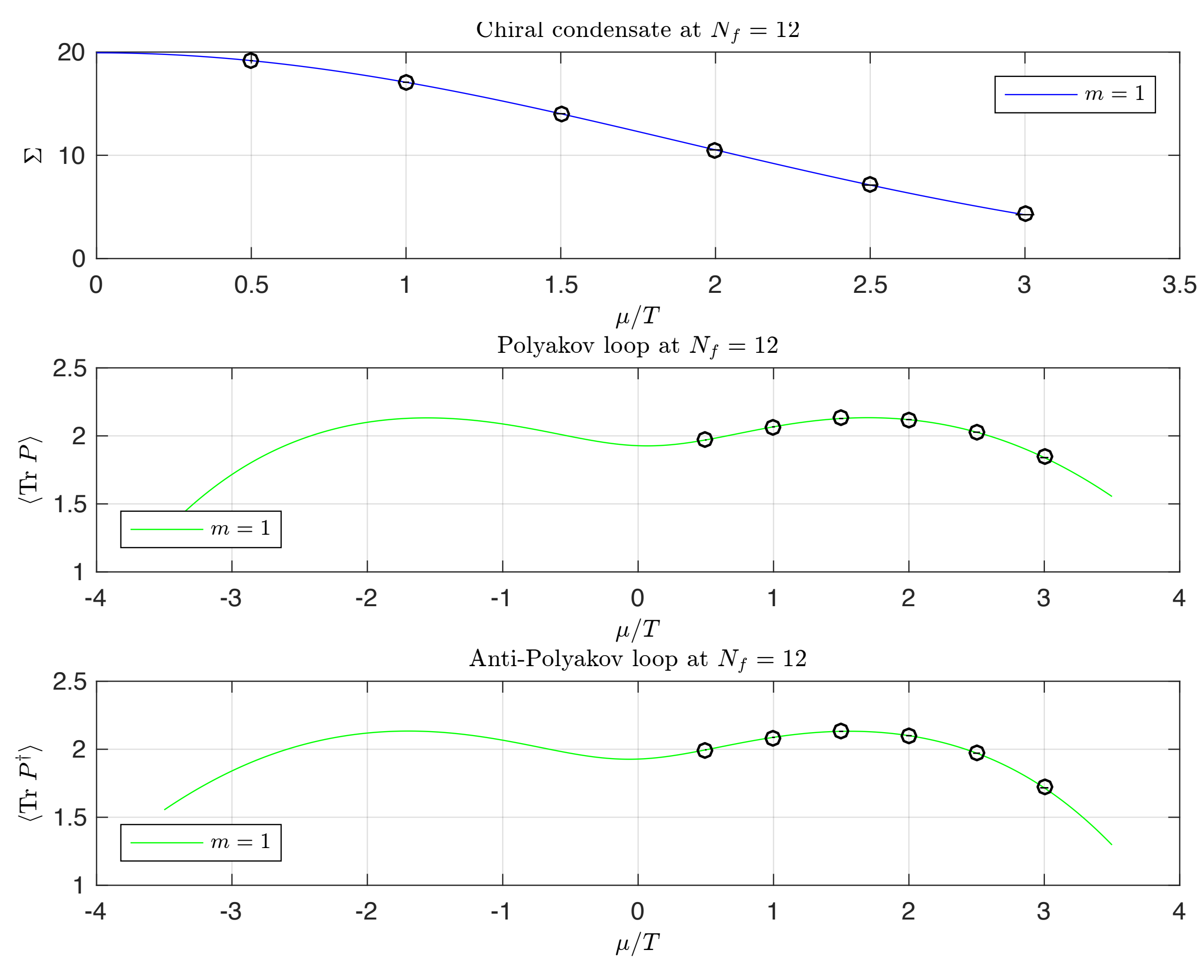
$$N_f\left\{B_\sigma^{-1}\left[\cosh\left(\frac{\mu}{T} + \frac{2\pi i\, k_\sigma}{3}\right) - 2B_\sigma^{-1}\sinh^2\left(\frac{\mu}{T} + \frac{2\pi i\, k_\sigma}{3}\right)\right]\right\} = \lambda_\sigma \, e^{i\,\varphi_\sigma}$$

These are interesting because we can predict the
relative weights of the different critical points!

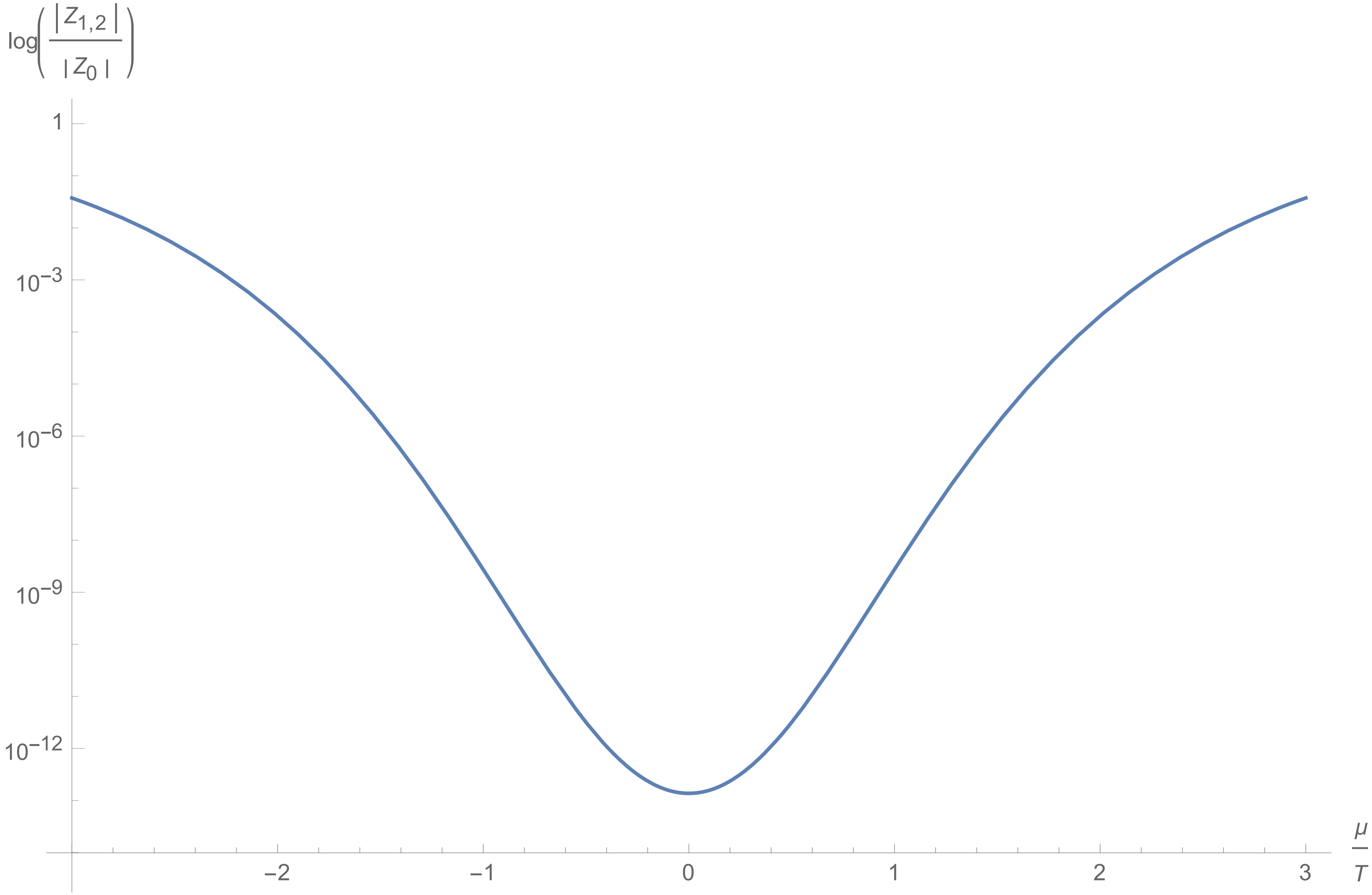
$N_f = 12$ $m = 0.1$



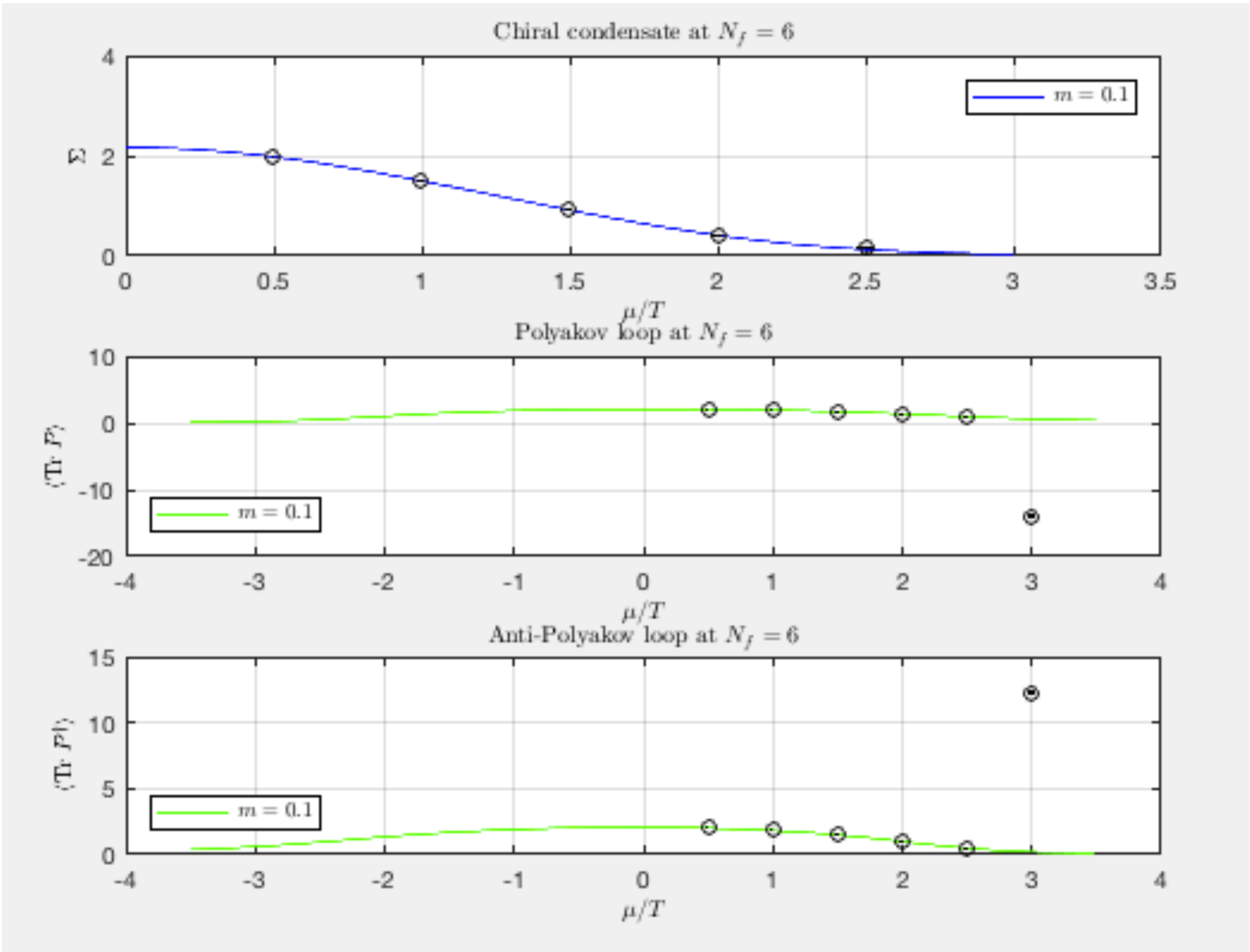
$N_f = 12$ $m = 1$



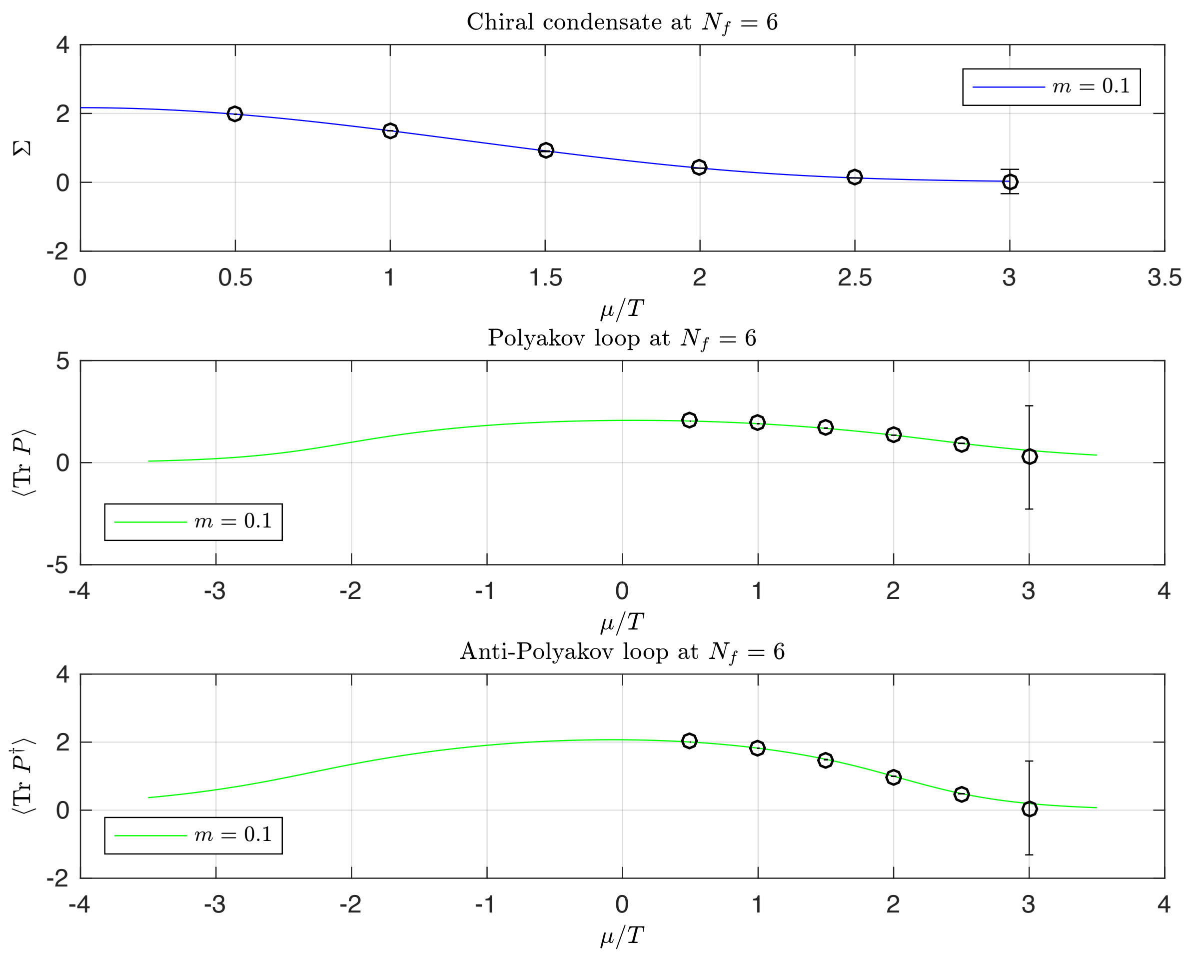
$N_f = 6$ $m = 0.1$ from semiclassical approximation



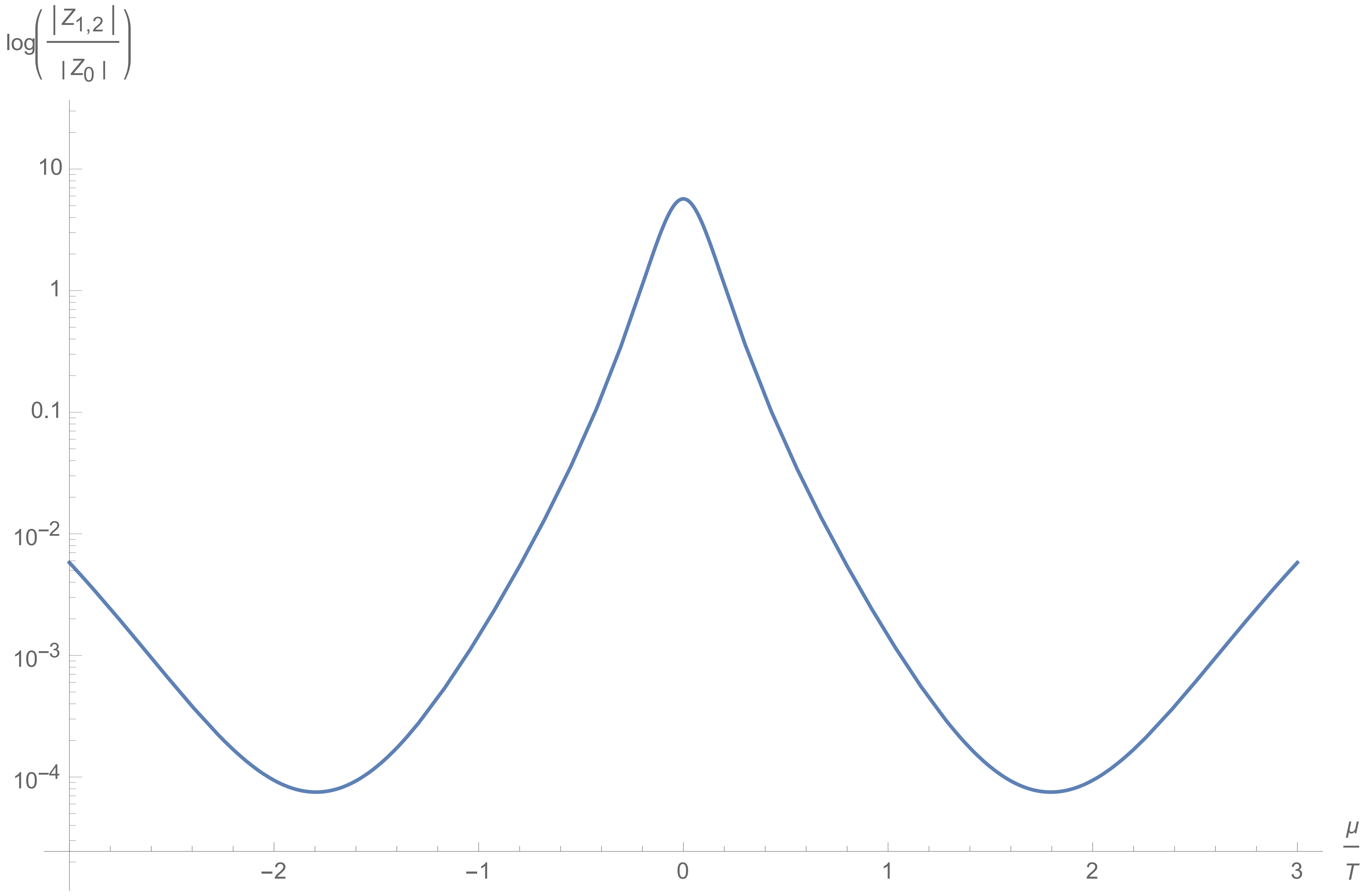
$N_f = 6$ m = 0.1



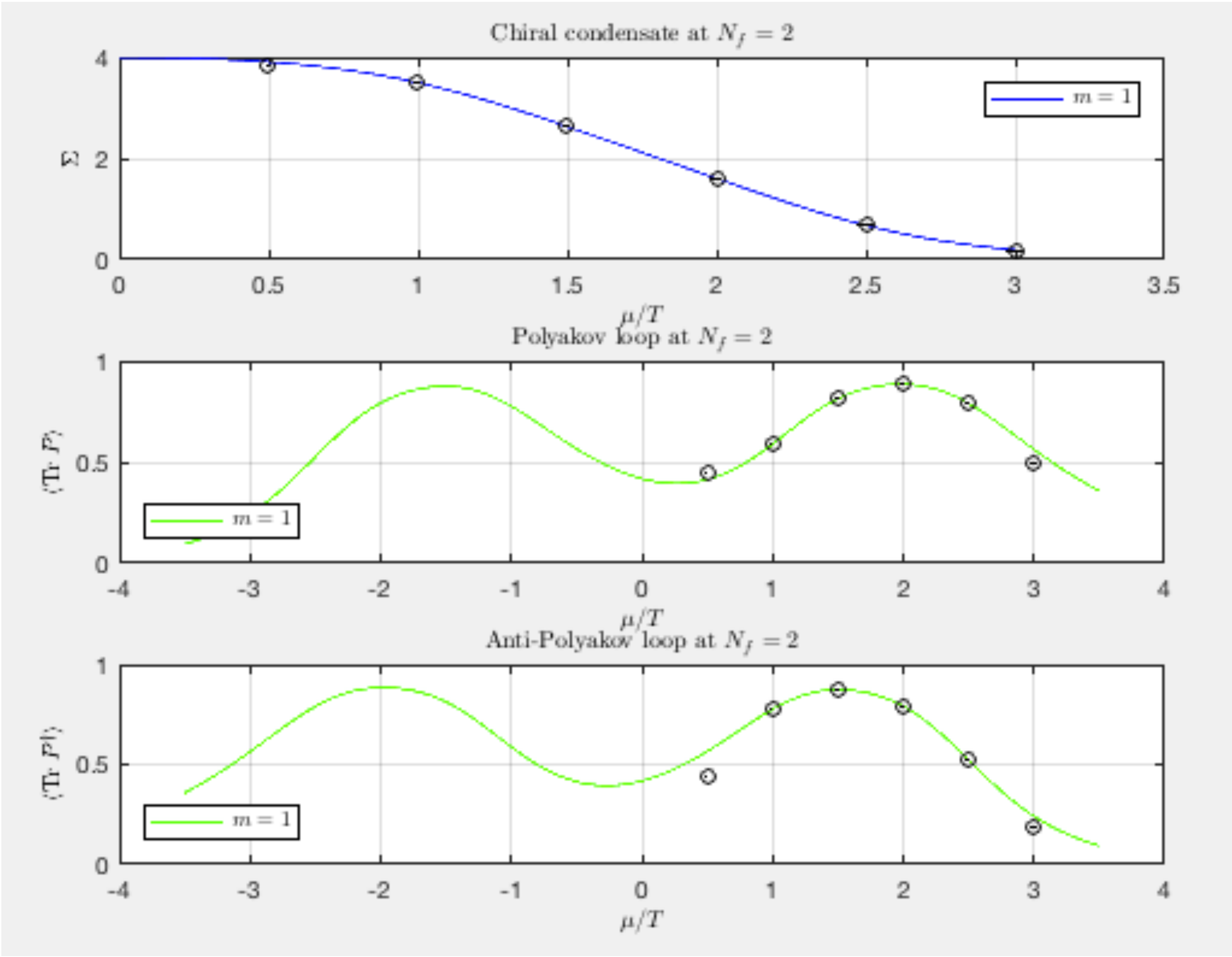
ONLY THIMBLE 0



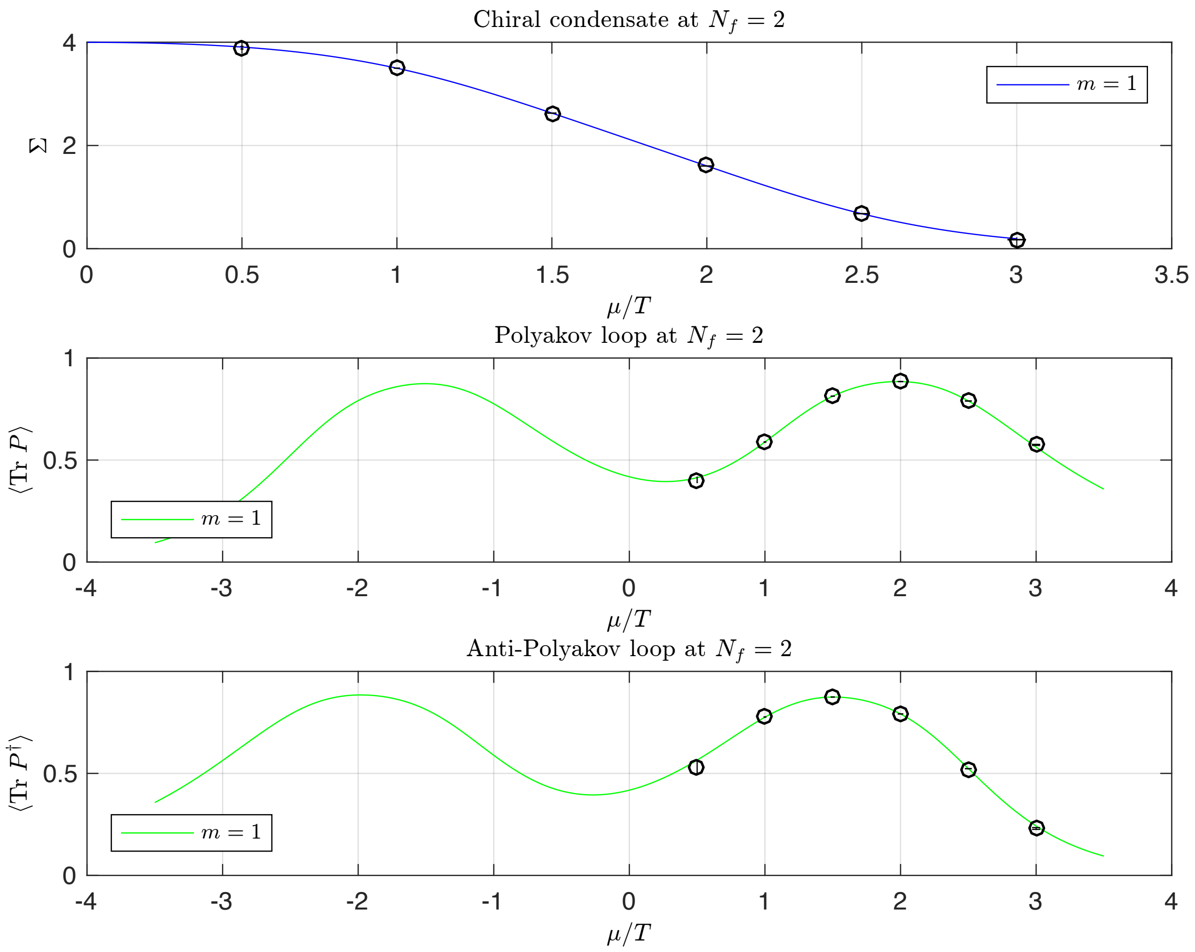
$N_f = 2$ $m = 1$ from semiclassical approximation



$N_f = 2$ $m = 1$

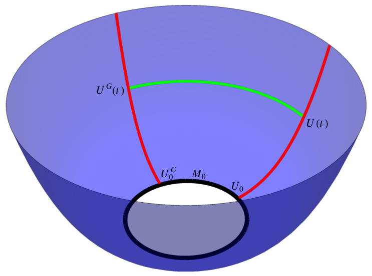


ONLY THIMBLE 0



The real thing: thimbles and the gauge structure of SU(N)

For gauge theories we need an improved picture for the thimble …



The relevant picture is that of a NON-DEGENERATE CRITICAL SUBMANIFOLD $\mathcal{N}$, for which

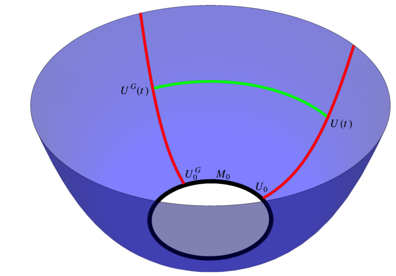
$$\mathcal{N} \subset \mathcal{C}$$

$$F : \mathcal{C} \to \mathbb{R}$$

$dF = 0$ along $\mathcal{N}$

The Hessian $\partial^2 F$ is non-degenerate on the normal bundle $\nu(\mathcal{N})$

For gauge theories we need an improved picture for the thimble …



The relevant picture is that of a NON-DEGENERATE CRITICAL SUBMANIFOLD $\mathcal{N}$, for which

$$\mathcal{N} \subset \mathcal{C}$$

$$F : \mathcal{C} \to \mathbb{R}$$

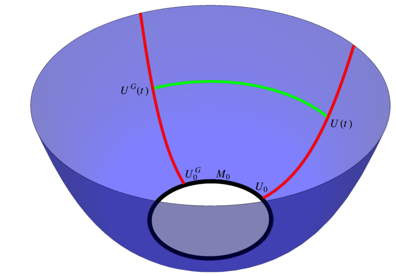
$dF = 0$ along $\mathcal{N}$

The Hessian $\partial^2 F$ is non-degenerate on the normal bundle $\nu(\mathcal{N})$

Let us consider QCD with its vacuum $A = 0$; $\mathcal{N}$ is the latter's complete gauge orbit

This is $SU(3)$ and the (real) dimension of the critical manifold is $(V-1)(N_c^2-1)$

For gauge theories we need an improved picture for the thimble …



The relevant picture is that of a NON-DEGENERATE CRITICAL SUBMANIFOLD $\mathcal{N}$, for which

$\mathcal{N} \subset \mathcal{C}$

$F : \mathcal{C} \to \mathbb{R}$

$dF = 0$ along $\mathcal{N}$

The Hessian $\partial^2 F$ is non-degenerate on the normal bundle $\nu(\mathcal{N})$

Let us consider QCD with its vacuum $A = 0$; $\mathcal{N}$ is the latter's complete gauge orbit

This is $SU(3)$ and the (real) dimension of the critical manifold is $(V-1)(N_c^2-1)$

In order to understand how the thimble will emerge, first observe that on the normal bundle we are provided with an equal number of positive and negative Takagi values of $\partial^2 F$ which are associated to the SD and SA flows.

Once again, in constructing thimbles we will be left with the right real dimension.

All in all, the thimble (e.g. associated to $A = 0$) is defined as

$$\mathcal{J}_0 := \Big\{ U \in (SL(3,\mathbb{C}))^{4V} \mid \exists U(\tau) \quad \text{solution of } \texttt{[*]} \mid U(0) = U \;\; \& \;\; \lim_{\tau \to \infty} U(\tau) \in \mathcal{N}^{(0)} \Big\}$$

$$\frac{d}{d\tau} U_\nu(x;\tau) = (-iT_a \overline{\nabla}_{x,\nu,a} \overline{S[U]}) U_\nu(x;\tau) \quad \texttt{[*]}$$

All in all, the thimble (e.g. associated to $A=0$) is defined as

$$\mathcal{J}_0 := \left\{ U \in (SL(3,\mathbb{C}))^{4V} \mid \exists U(\tau) \ \text{ solution of } \texttt{[*]} \mid \ U(0) = U \ \ \& \ \ \lim_{\tau\to\infty} U(\tau) \in \mathcal{N}^{(0)} \right\}$$

$$\frac{d}{d\tau} U_\nu(x;\tau) = (-i T_a \overline{\nabla}_{x,\nu,a} \overline{S[U]}) U_\nu(x;\tau) \quad \texttt{[*]}$$

A key point is now to understand that

under $SL(3,\mathbb{C})$ gauge transformations $\quad (T_a \overline{\nabla}_{x,\nu,a} \overline{S[U]}) \to \left(\Lambda(x)^{-1}\right)^\dagger (T_a \overline{\nabla}_{x,\nu,a} \overline{S[U]}) \Lambda(x)^\dagger$

$$U_\nu(x) \to \Lambda(x) U_\nu(x) \Lambda(x+\hat{\nu})^{-1}$$

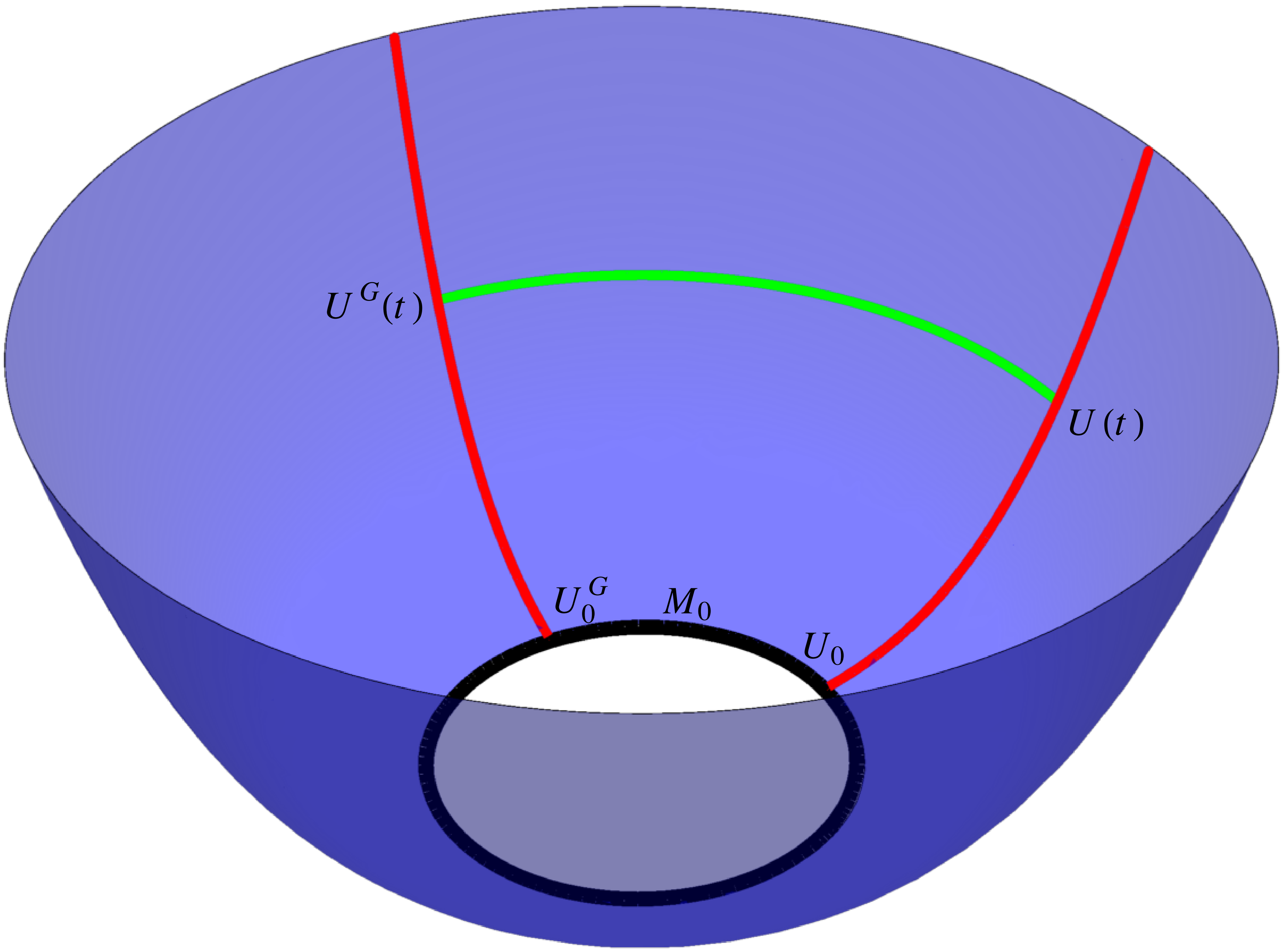
This not only means that the SD eq. is covariant only for $\Lambda(x)^\dagger = \Lambda(x)^{-1}$, i.e. $SU(3)$

... but also that if you take a SA from $A=0$, at any stage you can perform a g.transf.

and this will take you to a point starting from which under SD you are going to eventually

land on another point on the gauge orbit of $A=0$ (decided by the g. transf. you choose)

All in all, keep in mind this …



… and keep in mind that at each point of the gauge orbit of our vacuum the tangent space is spanned by both positive Takagi values of the Hessian (associated to the ascents) and null Takagi values (associated to gauge transformations)

Gaussian approximation for SU(N) (N=2 in d=2, actually)

A more realistic gauge theory
(although a somehow artificial sign problem)

$$S_G[U] = \beta \sum_{m\in\Lambda} \sum_{\hat{\rho}<\hat{\nu}} \left[1 - \frac{1}{2N} \mathrm{Tr} \left(U_{\hat{\rho}\hat{\nu}}(m) + U^{-1}_{\hat{\rho}\hat{\nu}}(m)\right)\right]$$

at complex values of the coupling

Hessian at the identity $\left.\nabla^b_{m,\hat{\rho}} \nabla^a_{n,\hat{\mu}} S_G[U]\right|_{U\equiv\mathbb{1}} =$

$$= \frac{\beta}{2N} \delta^{ab} \left[2D\delta_{n,m}\delta_{\hat{\mu},\hat{\rho}} - \delta_{n,m} + \delta_{n+\hat{\mu},m} + \delta_{n-\hat{\rho},m} - \delta_{n+\hat{\mu}-\hat{\rho},m} - \delta_{\hat{\mu},\hat{\rho}} \sum_{\hat{\nu}} (\delta_{n+\hat{\nu},m} + \delta_{n-\hat{\nu},m})\right]$$

has $d(N_c^2 - 1)$ extra zero modes, which do not come as a surprise: TORONS!

A more realistic gauge theory
(although a somehow artificial sign problem)

$$S_G[U] = \beta \sum_{m\in\Lambda} \sum_{\hat\rho<\hat\nu} \left[1 - \frac{1}{2N} \mathrm{Tr}\left(U_{\hat\rho\hat\nu}(m) + U^{-1}_{\hat\rho\hat\nu}(m)\right)\right]$$

at complex values of the coupling

Hessian at the identity $\nabla^b_{m,\hat\rho} \nabla^a_{n,\hat\mu} S_G[U]\big|_{U\equiv\mathbb{1}} =$

$$= \frac{\beta}{2N} \delta^{ab} \left[2D\delta_{n,m}\delta_{\hat\mu,\hat\rho} - \delta_{n,m} + \delta_{n+\hat\mu,m} + \delta_{n-\hat\rho,m} - \delta_{n+\hat\mu-\hat\rho,m} - \delta_{\hat\mu,\hat\rho} \sum_{\hat\nu} (\delta_{n+\hat\nu,m} + \delta_{n-\hat\nu,m})\right]$$

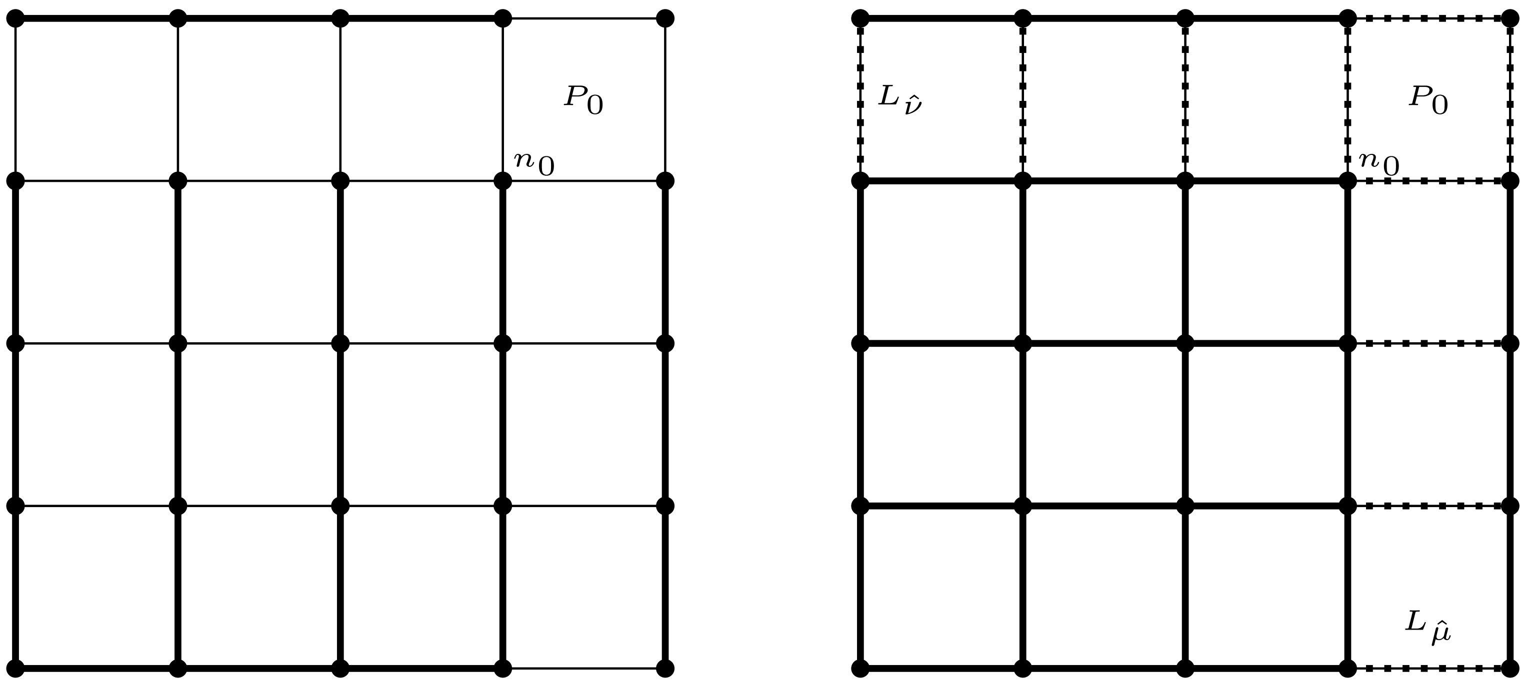
has $d(N_c^2 - 1)$ extra zero modes, which do not come as a surprise: TORONS!

Ok! Let's turn to a twisted action $S_G[U] = \beta \sum_P f_P^{(t)}(U_P)$

$$f_P^{(t)}(U_P) = \begin{cases} f_P(z_{\hat\mu\hat\nu} U_P) & P \in R_{\hat\mu\hat\nu} \\ f_P(U_P) & P \notin R_{\hat\mu\hat\nu} \end{cases} \qquad z_{\hat\mu\hat\nu} = e^{2\pi i n_{\hat\mu\hat\nu}/N} \in Z_N$$

We are playing around with this in its simplest form, i.e. d=2 and N_c=2. It is a nice laboratory: everything is known!

In order to proceed, first of all we have to recall what is the minimum action configuration once we have moved to the twisted action and chosen convenient twist.



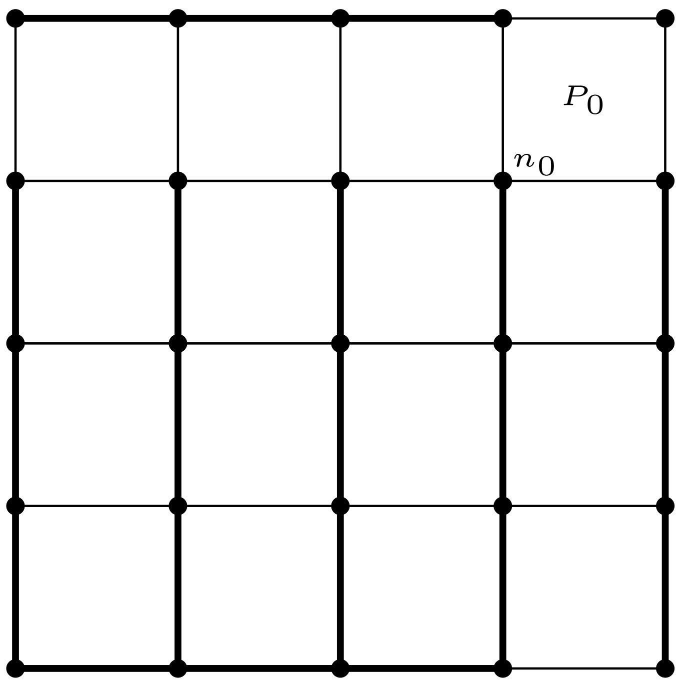
(a) Gauge tree (b) Zero action configurations

The construction of the gauge tree will remember many of you of classical literature on the subject, dating back to quite some time ago (Gonzalez-Arroyo, Korthals Altes, Van Baal, ...)

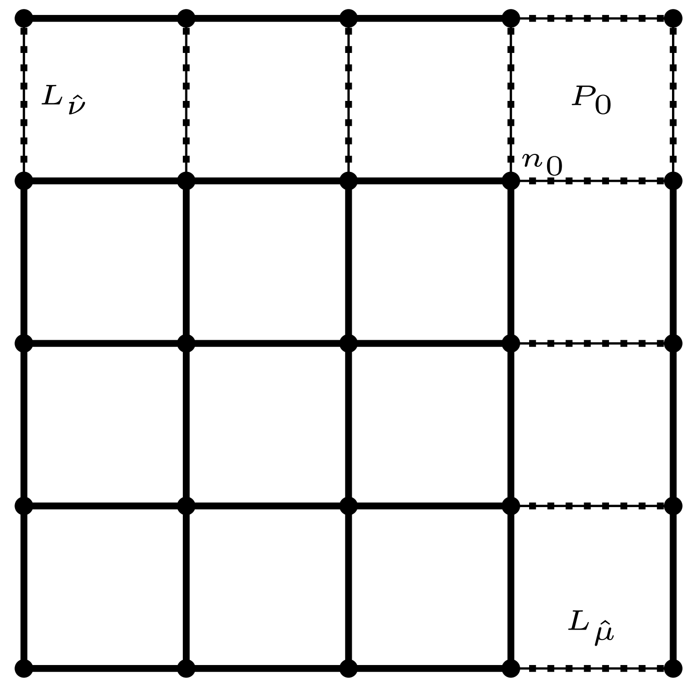
$$G_{\hat\nu} G_{\hat\mu} = z_{\hat\mu\hat\nu} G_{\hat\mu} G_{\hat\nu}$$

$$\mathcal{M}_0\left(z_{\hat\mu\hat\nu}\right) = \left\{ \left(G_1, \cdots, G_d\right) | G_{\hat\mu} \in \mathrm{SU}\left(N\right), G_{\hat\nu} G_{\hat\mu} = z_{\hat\mu\hat\nu} G_{\hat\mu} G_{\hat\nu} \right\} \qquad \dim \mathcal{N}_0 = \left(V-1\right)\left(N^2-1\right) + \dim \mathcal{M}_0\left(z_{\hat\mu\hat\nu}\right)$$

Twist-eater solution $\quad \dim \mathcal{M}_0 = N_c^2 - 1$



(a) Gauge tree



(b) Zero action configurations

The construction of the gauge tree will remember many of you of classical literature on the subject, dating back to quite some time ago (Gonzalez-Arroyo, Korthals Altes, Van Baal, ...)

$$G_{\hat{\nu}} G_{\hat{\mu}} = z_{\hat{\mu}\hat{\nu}} G_{\hat{\mu}} G_{\hat{\nu}}$$

$$\mathcal{M}_0\left(z_{\hat{\mu}\hat{\nu}}\right) = \left\{\left(G_1, \cdots, G_d\right) | G_{\hat{\mu}} \in \mathrm{SU}\left(N\right), G_{\hat{\nu}} G_{\hat{\mu}} = z_{\hat{\mu}\hat{\nu}} G_{\hat{\mu}} G_{\hat{\nu}}\right\} \qquad \dim \mathcal{N}_0 = \left(V-1\right)\left(N^2-1\right) + \dim \mathcal{M}_0\left(z_{\hat{\mu}\hat{\nu}}\right)$$

Twist-eater solution $\quad \dim \mathcal{M}_0 = N_c^2 - 1$

With this we can construct a thimble to start with: in particular we can identify the tangent space at the critical point (in the critical orbit …). We find the expected number of positive Takagi values to the Hessian (the associated Takagi vectors define directions for ascents) and null Takagi values (the associated Takagi vectors define directions for the gauge transformations taking you along the orbit).

Given a thimble formulation, our first attempt will be to test the validity of what we call the gaussian approximation.

The gaussian approximation

First of all observe that Langevin is the natural candidate to simulate on a thimble!

$$\frac{d}{d\tau}\phi_{a,x}^{(R)} = \boxed{-\frac{\delta S_R}{\delta \phi_{a,x}^{(R)}}} + \eta_{a,x}^{(R)}$$

$$\frac{d}{d\tau}\phi_{a,x}^{(I)} = \boxed{-\frac{\delta S_R}{\delta \phi_{a,x}^{(I)}}} + \eta_{a,x}^{(I)}$$

On the thimble by very definition!

Noise should be tangent to the thimble!

The gaussian approximation

First of all observe that Langevin is the natural candidate to simulate on a thimble!

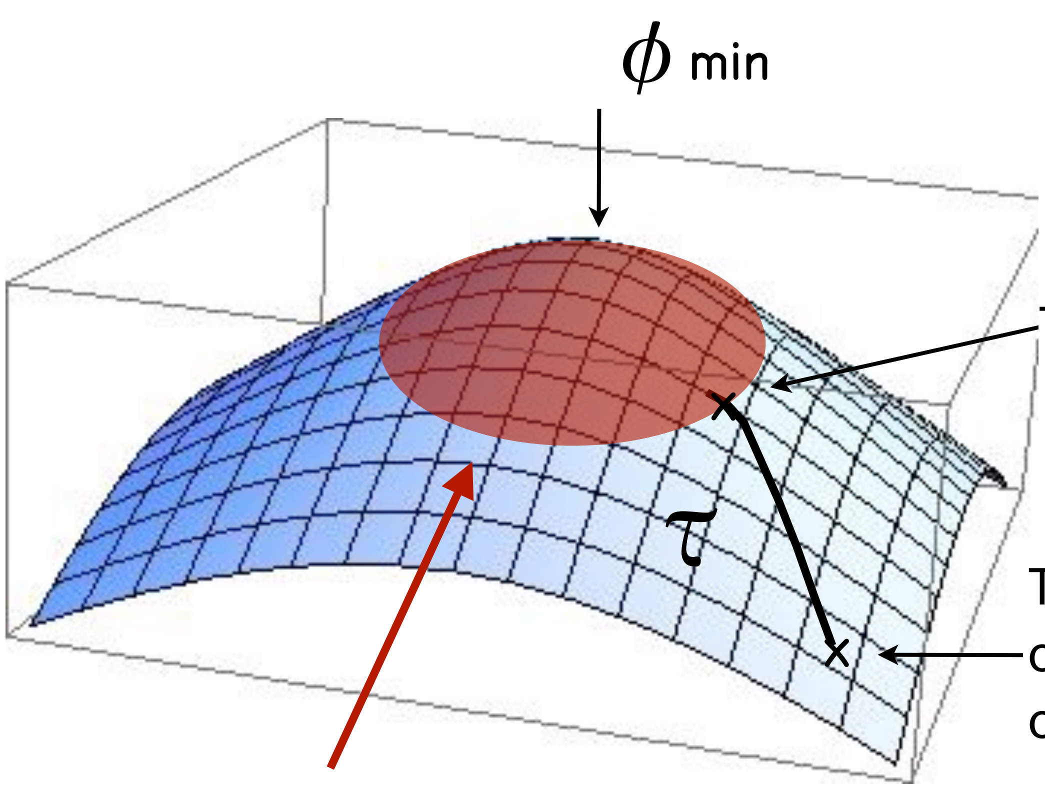
$$\frac{d}{d\tau}\phi^{(R)}_{a,x} = \boxed{-\frac{\delta S_R}{\delta\phi^{(R)}_{a,x}}} + \eta^{(R)}_{a,x}$$

$$\frac{d}{d\tau}\phi^{(I)}_{a,x} = \boxed{-\frac{\delta S_R}{\delta\phi^{(I)}_{a,x}}} + \eta^{(I)}_{a,x}$$

On the thimble by very definition!

Noise should be tangent to the thimble!

But we easily know what the tangent is only (at) near the critical point!



This point is at the border …

This point sits on the flow line well beyond the border of the region where the tangent space almost sits on top of the tangent space at the critical point …

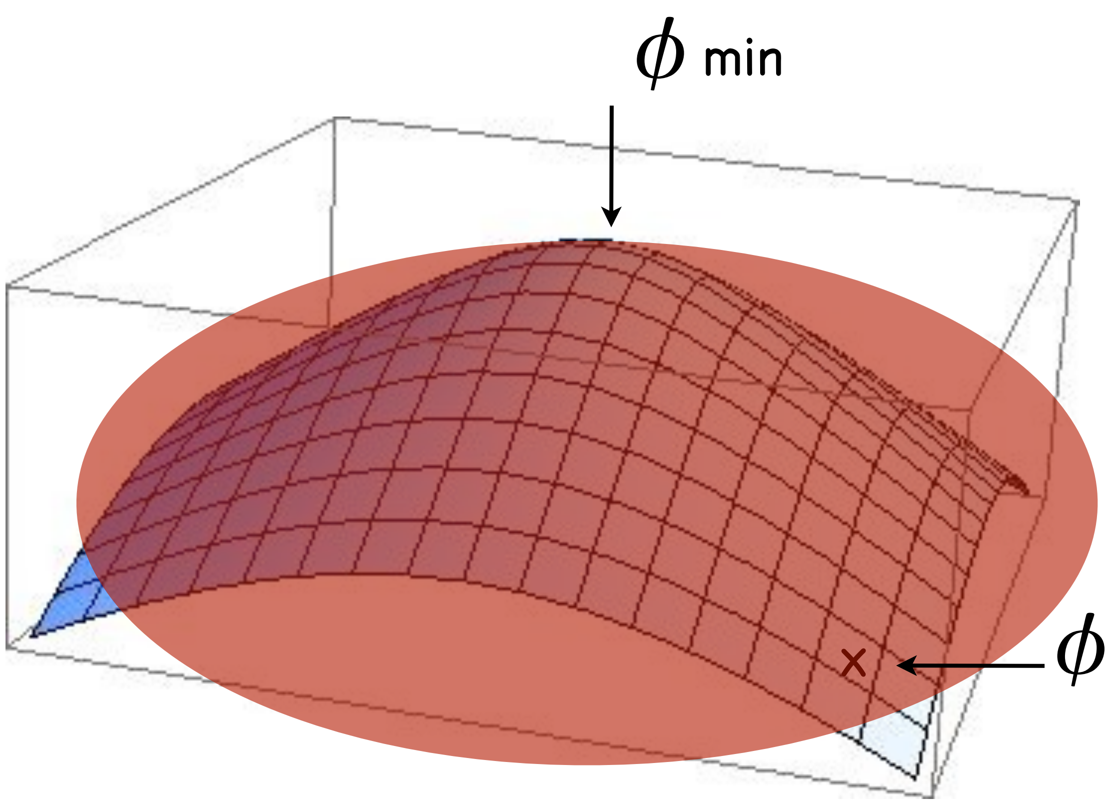
Region of applicability of the Hessian computed in ϕ min

The gaussian approximation (as crude as it is … Bose gas ok! AuroraColl. PRD88)

$$\frac{d}{d\tau}\phi_{a,x}^{(R)} = \boxed{-\frac{\delta S_R}{\delta\phi_{a,x}^{(R)}}} + \eta_{a,x}^{(R)}$$

$$\frac{d}{d\tau}\phi_{a,x}^{(I)} = \boxed{-\frac{\delta S_R}{\delta\phi_{a,x}^{(I)}}} + \eta_{a,x}^{(I)}$$

On the thimble by very definition! Noise is on the tangent space at the crit. point!



But there can be cases in which the relevant region for the functional integral can be deformed to end up on top of the tangent space at the critical point (think of saddle point).

We call this gaussian approximation because the thimble and the tangent space at the critical point are the same for a theory having only quadratic contributions on top of the value at the critical point (think of the saddle point approximation): in such a case the thimble is flat.

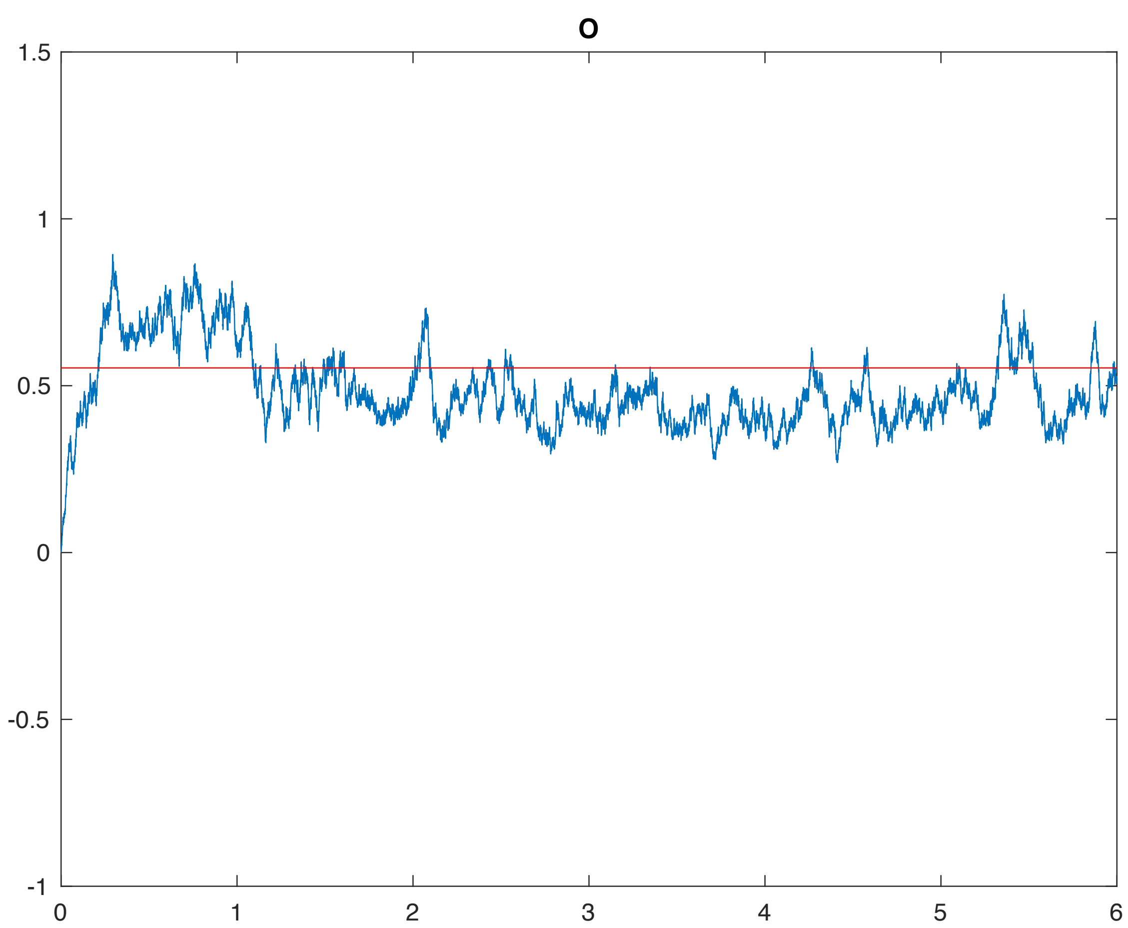
Recently A. Alexandru et al have introduced a similar approach to the computation on what they call the main tangent space (JHEP 1605 053).

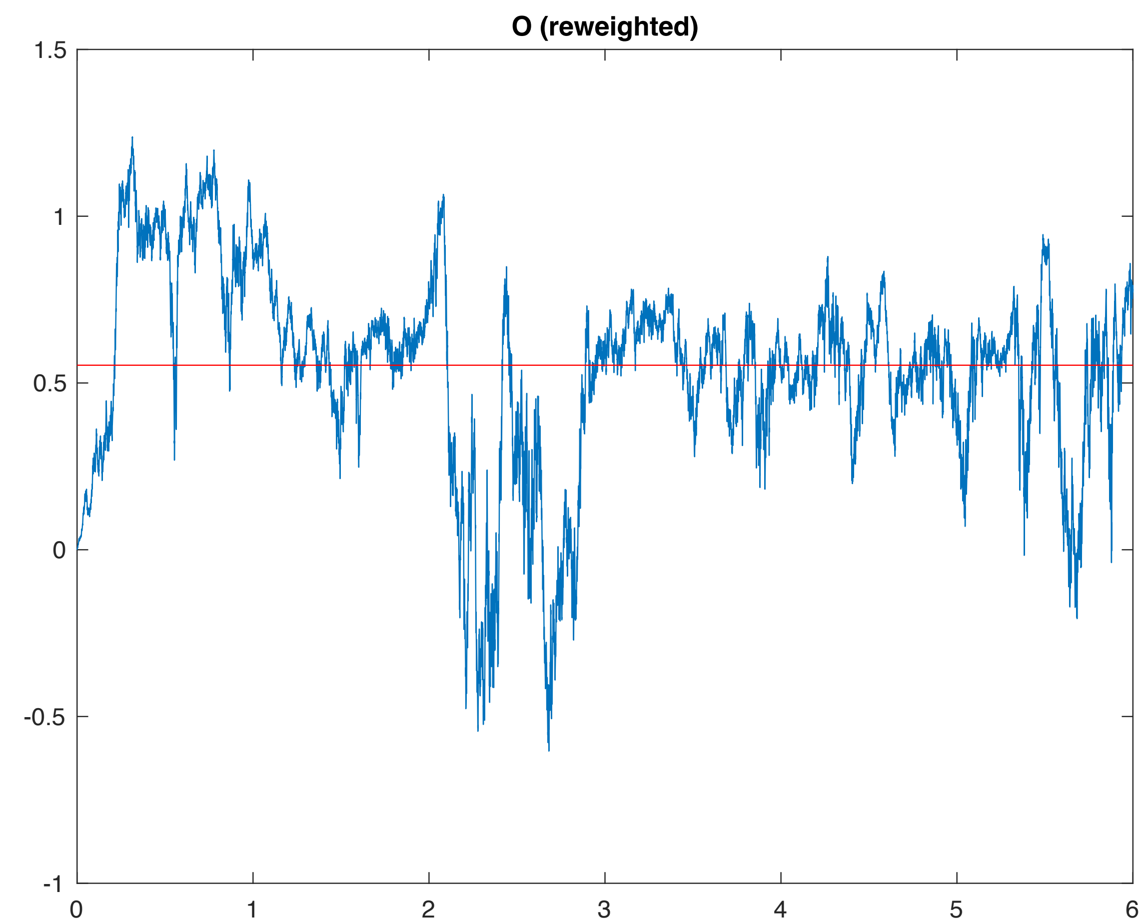
Not that bad …

$$SU(2) \qquad d = 2 \qquad \beta = 5\,e^{i\,0.2}$$

Semiclassical approximation suggests gaussian approximation should be reasonably ok …

We measure the action density. Caveat: everything very very preliminary!





Conclusions

- We have a new Monte Carlo for thimbles in terms of complete flow lines.

- Basic formalism for lattice gauge theories is alive and kicking for QCD 0+1.

- SU(2) in d=2 apparently under control in the gaussian approximation in a region where it should be under control.

- A HUGE amount of WORK yet to be done … !