

Thimble regularisation of YM fields: crunching a hard problem

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Thimble regularisation of Yang Mills theories is still to a very large extent terra incognita. We discuss a couple of topics related to this big issue. 2d YM theories are in principle good candidates as a working ground. An analytic solution is known, for which one can switch from a solution in terms of a sum over characters to a form which is a sum over critical points. We would be interested in an explicit realisation of this mechanism in the lattice regularisation, which is actually quite hard to work out. A second topic is the inclusion of a topological term in the lattice theory, which is the prototype of a genuine sign problem for pure YM fields. For both these challenging problems we do not have final answers. We present the current status of our study.

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1. A thimble primer

QCD at finite baryon density is still to a large extent *terra incognita*, due to the infamous sign problem. The latter is in fact more general (and fundamental, in a sense): we have to tackle it every time the action of a quantum field theory is complex valued. A number of possible solutions have been put forward, among which thimble regularisation [1, 2]. In a light notation in which a field theory looks like an ordinary integral, the thimble approach to field theories is quite easy to describe in terms of the following recipes:

1. We first need to complexify the degrees of freedom, *i.e.* $x \rightarrow z = x + iy$ and $S(x) = S^R(x) + iS^I(x)$ ¹ $\rightarrow S(z)$.
2. We then need to find the critical points, *i.e.* those points p_σ where $\partial_z S = 0$.
3. We define the thimble \mathcal{J}_σ attached to each critical point as the union of all the Steepest Ascent paths (SA), the latter being the solutions of $\frac{d}{dt} z_i = \frac{\partial S}{\partial \bar{z}_i}$ stemming from the critical point.
4. If the Hessian of the action has no zero eigenvalue, one can immediately prove that the thimble is a manifold of the same real dimension as the original manifold we started from.
5. Due to the holomorphic nature of S , S^R is increasing along the ascent and thus on the thimble the original integral is convergent, while S^I stays constant.
6. Sadly, the sign problem is *not completely* killed, since the integration measure (encoding the orientation of the thimble with respect to the embedding manifold) reintroduces a *residual* sign problem due the so-called *residual phase*.

The last point would deserve much more attention than we can pay here; the interested reader can look at [3] for our (basic, but stemming from first principles) solution to the computation of the residual phase. While going through all the steps needed to carry out a computation on thimbles can be a non trivial task, our efforts are fully rewarded by Lefschetz/Picard theory, which states that a thimble decomposition for the original path integral holds

$$\langle O \rangle = \frac{\sum_\sigma n_\sigma e^{-iS^I(p_\sigma)} \int_{\mathcal{J}_\sigma} dz e^{-S^R} O e^{i\omega}}{\sum_\sigma n_\sigma e^{-iS^I(p_\sigma)} \int_{\mathcal{J}_\sigma} dz e^{-S^R} e^{i\omega}} \quad (1)$$

In (1) S^I is no longer such a big problem, while the residual sign problem is due to the residual phases $e^{i\omega}$. Notice that both the numerator and the denominator (*i.e.* the partition function) receive contributions in principle by all the critical points. This is not really the case, since the *intersection numbers* n_σ can be zero for possibly many critical points. It can be shown that $n_\sigma = 0$ for a critical point when the associated *unstable* thimble does not intersect the original integration manifold².

¹It is important to remind that the action is complex since the very beginning, even for real degrees of freedom.

²The unstable thimble is defined as the union of the Steepest Descent (SD) paths stemming from a critical point.

2. Thimble regularisation of gauge theories

We started our discussion on motivations for thimbles putting forward the big issue of QCD at finite density. How far are we from actually tackling that? Honestly, quite a lot. We have in recent years taken some steps in that direction, but that has been done in the context of two theories (0 + 1 QCD [4] and the so called *Heavy Dense QCD* [5]) for which gauge invariance in practice does not show up in its full glory. Other groups have perhaps moved a bit further than we have done till now [6, 7]. In the following we will try to pin down a sort of status report on our attempts at a thimble regularisation of gauge theories. This will make us discuss 2D YM theories and the inclusion of a θ -term.

2.1 Construction of the thimble

Mimicking thimble construction for gauge theories is not that difficult. The first step (complexification) amounts to

$$\mathrm{SU}(N) \ni U = e^{ix_a T^a} \rightarrow e^{iz_a T^a} = e^{i(x_a + iy_a) T^a} \in \mathrm{SL}(N, \mathbb{C}). \quad (2)$$

The main thing we should notice is that

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

With this caveat in mind, we can proceed to defining the SA

$$\frac{d}{d\tau} U_{\hat{\mu}}(n; \tau) = \left(i T^a \bar{\nabla}_{n, \hat{\mu}}^a \overline{S[U(\tau)]} \right) U_{\hat{\mu}}(n; \tau) \quad (3)$$

which are written in terms of the Lie derivative

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

Notice that, since $\frac{d}{d\tau} = \bar{\nabla}_{n, \hat{\mu}}^a \bar{S} \nabla_{n, \hat{\mu}}^a + \nabla_{n, \hat{\mu}}^a S \bar{\nabla}_{n, \hat{\mu}}^a$ we have that

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

and

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

that is, the main properties we expect from the SA are satisfied. Among all the solutions of Eq. (3), we have to look for the ones whose union defines the thimble. Naively, we could think we need to consider those stemming from a critical point U_σ . The fact is critical points in gauge theories come along with an entire orbit, which is made by all the gauge replicas of the given critical point. This is not the end of the story, since complexification has left us with two possible candidates. The action is now invariant under the gauge group $\mathcal{G} = \mathrm{SL}(N, \mathbb{C})$, so that one orbit we could think of is

$$\mathcal{M}_\sigma = \{U \in \mathrm{SL}(N, \mathbb{C}) \mid \exists G \in \mathrm{SL}(N, \mathbb{C}) : U_\sigma^G = U\}.$$

This is not the right choice, and we need to consider instead

$$\mathcal{N}_\sigma = \{U \in SL(N, \mathbb{C}) \mid \exists G \in SU(N) : U_\sigma^G = U\} \subset \mathcal{M}_\sigma. \quad (4)$$

In general the relevant gauge group is $\mathcal{H} = SU(N)$, and as a matter of fact the thimble itself is invariant under $SU(N)$ (as it should be), and not under $SL(N, \mathbb{C})$. All in all, the thimble *e.g.* associated to $A = 0$ for the $SU(3)$ Yang-Mills action is defined by³

$$\mathcal{J}_0 := \left\{ U \in (SL(3, \mathbb{C}))^{4V} \mid \exists U(\tau) \text{ solution of Eq. (3)} \mid U(0) = U \ \& \ \lim_{\tau \rightarrow -\infty} U(\tau) \in \mathcal{N}^{(0)} \right\}. \quad (5)$$

One could think that what we have gone through till now can be summarised as “going from critical points to critical submanifold”. We have to admit we have been cheating a little bit: what we actually did (and this is actually the right thing to do) was to go from *non-degenerate* critical points to *non-degenerate* critical submanifolds [8]. In Sec. 1 we said that in order for the thimble construction to work we need a non-degenerate critical point, with no zero eigenvalue in the Hessian. Due to gauge modes, this is not the case for gauge theories. The good news is that this is not such a big problem: gauge invariance is realised in a very neat way on the thimble. Indeed the main gauge invariant property of the construction is summarised in the cartoon⁴ of Fig 1. One can spot

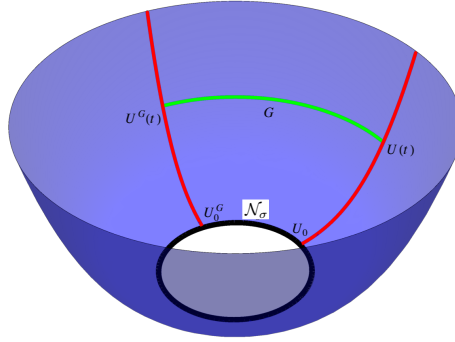


Figure 1: The cartoon for the gauge invariance property of the construction of Eq. 5.

the point $U(t)$ which is obtained by ascending from the critical point U_0 ⁵: this point is uniquely defined by selecting a given direction on the tangent space to the thimble at U_0 ⁶ and a given ascend time t . Ascent paths of this type are defined selecting directions associated to positive eigenvalues of the Hessian. As for (zero) gauge modes, their role is well understood by looking at the point $U^G(t)$. All in all, if we take a SA from U_0 (*i.e.* $A = 0$), at any stage (*i.e.* from any $U(t)$) we can perform a gauge transformation G and this will take us to a point ($U^G(t)$) starting from which the SD (Steepest Descent) path will make us eventually land on another point on the gauge orbit attached to U_0 ; this point (U_0^G) is obtained from U_0 by the gauge transformation we choose.

³We denote $\mathcal{N}^{(0)}$ the orbit \mathcal{N}_σ associated to $A = 0$.

⁴We provide a quick-and-dirty argument for what a non-degenerate critical submanifold is; all this can be much better understood from [8].

⁵We are still thinking of the critical point $A = 0$, which in the Wilson action is associated to its exponential U_0 .

⁶This is always known by solving a convenient Takagi problem; see [3].

All that we have said till now is not the end of the story, and we have been once again cheating a little bit. In order to preserve the right number of zero modes, in YM theories we have to kill *torons*, which thing can be done by going for twisted boundary conditions. Because of this, our preferred critical point is the so-called *twist-eater*. (A good reference for all that has to do with this is [9].)

2.2 What we have, what we can do and what we lack

We have a (working) code (some results in Fig. 2) by which we can simulate 2D YM theories; to be definite, we have been mainly focusing on $SU(2)$. A sign problem (an artificial one, in a sense) is generated by computing for complex values of the coupling. Notice that the theory is fully solved, so that we can check the results we get. One thing we do is *hunting for critical points*, the main goal being to compute on different thimbles. This is in the logic of (dis)proving whether one single thimble is enough to reproduce the known result (and this indeed appears not to be the case: see Fig. 2).

In all that we have just mentioned there is indeed something we (dramatically) miss: *there is no general proof of something like a thimble decomposition for gauge theories*. This is the genuine motivation of ours for probing 2D YM theories: the solution is known in a way that is intriguing, sort of *alluding* to thimbles.

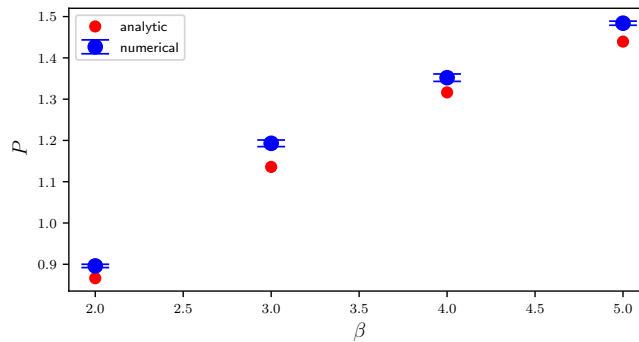


Figure 2: Average Plaquette vs real β for the numerical (only dominant thimble) vs analytical results for 2D $SU(2)$ YM theory.

2.3 The closest to thimble decomposition for gauge theories we can currently think of getting

Indeed we think 2D YM theories provides us with an understanding which is *the closest to thimble decomposition for gauge theories we can currently think of getting*. What we mean is displayed (once again) in graphical form in Fig. 3. For a full account of the results we are going to quote a first reference is [10]. First of all look at the first row of Fig. 3. All the critical points that are classical solutions of the YM action have been classified by Atiyah and Bott in [8]. In [10] Witten first obtains the partition function as a sum over representations (this is a type of result which is well known to lattice practitioners; see later) on a generic Riemann surface of *genus* g , which for $g = 1$ reduces to the expression in the up-left corner of Fig. 3. Via a tool as simple as the *Poisson resummation*, he then turns this sum into a sum over critical points (up-right corner). Needless to say, this is the intriguing result we are mostly interested in: this really *sounds like thimble decomposition*. Now look at the second row. Down-left corner of Fig. 3 is the sum over

$$\begin{array}{ccc}
 \sum_{n \in \mathbb{Z}} \exp(-\epsilon \pi^2 n^2) & \xrightarrow{\text{Poisson resummation}} & \sum_{m \in \mathbb{Z}} \exp\left(\frac{-(2\pi m)^2}{\epsilon'}\right) \\
 \uparrow \text{continuum limit} & & \uparrow ? \\
 Z^{(pbc)}(\beta) = e^{-\beta V} \sum_{n=1}^{\infty} \left[\frac{2}{\beta} I_n(\beta) \right]^V & \xrightarrow{?} & ?
 \end{array}$$

Figure 3: The flow chart of a possible argument in favor of thimble decomposition in $2D$ $SU(2)$ YM theory.

representation which is well known to the lattice community, *i.e.* the Migdal solution [11]. It is well known that one can take the continuum limit and go from down-left to up-left [12]. Finally, what we regard as the big issue: can we fill the down-right corner, *i.e.* provide a realisation of the mechanism in the first row in the lattice regularisation? The complete task would entail taking the continuum limit and go from down-right to up-right.

3. Looking into θ -term

While we have been working on $2D$ YM theories, we have adapted our code to also include $4D$ YM in the presence of a θ -term. Once again we do not have yet definite results, but it is easy to list a few reasons for being interested in this.

- This is a prototype of a *genuine* sign problem in Euclidean Yang Mills.
- Being the equations of motion unaffected by a θ -term, the topological charge is conserved while you ascent on the thimble; in a way, this is a genuine way of computing at frozen topological charge.
- We have already made the point that the gauge invariance of the thimble is that of $SU(N)$; this holds for the topology as well.
- All in all, the really intriguing (super-hard!) goal would be that of finding the weights of the various topological sectors in the functional integral.

Needless to say, one should be well aware of the effects of lattice artifacts (they must show up, as in any lattice computations of topology). And of course, all this is indeed interesting, but it is not at all guaranteed that we can get positive results in a short time.

4. Conclusions

We have provided a status report of our attempts at formulating gauge theories on thimbles. We do not have positive results to present, but we have a couple of lines of research that are hard to crunch, but fascinating. We would like to find a lattice realisation of the mechanism that in $2D$ gauge theories enables to go from a solution in terms of a sum over characters to a form which is a sum over critical points. $4D$ YM in the presence of a θ -term is a second subject which is rich of interesting features to investigate.

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