Thimble regularization of finite density field theories: a primer/update

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Thimble regularization of field theories (M. Cristoforetti, F. Di Renzo, L. Scorzato - Phys.Rev.D88 2013) is still a fairly new attempt at the solution of the infamous sign problem.

I will mostly provide a sketch of the status of our studies, taking this also as a chance to present some still unpublished material which has to do with a (quite famous, actually) toy model. The latter will in a sense guide us, introducing problems and opportunities.

**Agenda**

- **Stumbling into thimbles: motivations** (including how it all began)

- **A few basic definitions and the overall scenario:** QFT on (a) thimble(s)

- A (very basic) example to make your way into the subject
  (including algorithmic issues)

- Where we stand
Stumbling into thimbles: motivations (including how it all began)
To introduce our approach, observe that strongly oscillating, low dimensional integrals are treated very effectively with the

\[ \text{Ai}(x) := \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\left(\frac{t^3}{3} + xt\right)} \, dt \quad \text{vs} \quad \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\left(\frac{z^3}{3} + xz\right)} \, dz \rightarrow \frac{1}{2\pi} e^{i\phi} \int_{\gamma} e^{R[i\left(\frac{z^3}{3} + xz\right)]} \, dz \]

A few remarks:

- Most often seen in its asymptotic expansion form
- It combines stationary phase and localization of important contributions
- The latter are very good candidates to tackle the sign problem!
How it all began (inspiration from E. Witten 2010)

Witten’s concern

- Extending the definition of the path integral for a few theories

Our concern

- For lattice finite density problems, Z is well defined, but the theory can not be sampled by MonteCarlo ...

There is a full generalization of saddle point by means of Lefschetz thimbles (and a sistematic framework within MORSE THEORY)

See the set of thimbles a combination of which (with integer coefficients) makes the job for any domain of integration for the Airy integral.
A few basic definitions and the overall scenario: QFT on (a) thimble(s)
A Summa of fundamental results from Morse Theory

The generalization of Steepest Descent paths are known as LEFSCHETZ THIMBLES $\mathcal{J}_\sigma$

in terms of which

$$\int_C dx \ g(x)e^{f(x)} = \sum_{\sigma} n_\sigma \int_{\mathcal{J}_\sigma} dz \ g(z)e^{f(z)} \quad C = \sum_{\sigma} n_\sigma \mathcal{J}_\sigma$$

Valid under suitable conditions on $f(x)$ and $g(x)$ and where

- The greek index $\sigma$ is attached to stationary points $p_\sigma$ of the complex(ified) $f(z)$
- $\mathcal{J}_\sigma$ is the union of all the SD paths that fall into $p_\sigma$ at infinite time
- $n_\sigma = \langle C, K_\sigma \rangle$ are the intersection numbers ...
- ... of the original domain with the dual thimbles $K_\sigma$ union of Steepest Ascent

Everything comes with the right (real) dimension!
... but having said this, we state since the very beginning that

the fundamental idea remains that of attempting a formulation of quantum field theories on Lefschetz thimbles (i.e. on SD paths in the complexified theory), maybe without trying to reconstruct the original integral via Morse Theory results.

In other terms, it is intriguing to take into account from the very beginning a scenario in which

\[ C = \sum_{\sigma} n_\sigma J_\sigma \quad \rightarrow \quad J_0 \]
A (very basic) example to make your way into the subject
A (quite old, actually) toy model

\[ S(\phi) = \frac{1}{2} \sigma \phi^2 + \frac{1}{4} \lambda \phi^4 \]

with \( \phi \in \mathbb{R}, \lambda \in \mathbb{R}^+ \) and \( \sigma = \sigma_R + i \sigma_I \in \mathbb{C} \).

\[ \langle \phi^n \rangle = \frac{1}{Z} \int_{\mathbb{R}} d\phi \, \phi^n \, e^{-S(\phi)} \quad Z = \int_{\mathbb{R}} d\phi \, e^{-S(\phi)} \]

This is a prototypal toy model for a field theory displaying a sign problem. Since the (quite old) paper by J. Ambjorn (Phys.Lett.B 1985) it has been attracting attention ...

... in part because of the problematic convergence properties of Complex Langevin. See Arts, Giudice, Seiler, Ann. Phys. 337 2013: good convergence properties only in a region of parameters space (not all the momenta can be computed).

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Thimbles in practice ...

\[ \phi = x + iy \]
\[ \phi_0 = 0 \]
\[ \phi_\pm = \pm \sqrt{-\frac{\sigma}{\lambda}} \]

\[ \begin{aligned}
\frac{dx}{dt} &= -\frac{\partial S^R(x,y)}{\partial x} \\
\frac{dy}{dt} &= -\frac{\partial S^R(x,y)}{\partial y}
\end{aligned} \quad \phi_\sigma \text{ for } t \to +\infty \]

\[ \langle \phi^n \rangle = \frac{1}{Z} \sum_\sigma m_\sigma e^{-iS^I(\phi_\sigma)} \int_{\mathcal{J}_\sigma} d\phi \phi^n e^{-S^R(\phi)} \]

\[ H(x,y) = \begin{pmatrix} \sigma_R + 3\lambda x^2 - 3\lambda y^2 & -\sigma_I - 6\lambda xy \\ -\sigma_I - 6\lambda xy & -\sigma_R - 3\lambda x^2 + 3\lambda y^2 \end{pmatrix} \]
A rich scenario ...
A rich scenario ...

A continuity argument tells you the correct combinations of weights!

\[ Z[\sigma_R \to 0^+] = Z[\sigma_R \to 0^-] = Z[\sigma_R = 0] \]
Field theories?!

\[ \mathcal{C} = \sum_{\sigma} n_\sigma \mathcal{J}_\sigma \rightarrow \mathcal{J}_0 \]

Being (much...) richer may be the path to simplicity!

- **Universality**: a single thimble can give a FT formulation with the same degrees of freedom, the same symmetries and symmetry representations, the same PT and naive continuum limit of the original formulation: good enough!

And moreover

- In the thermodynamic limit a simple argument (supported by Morse theory) suggests that only the thimbles attached to global minima can survive

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Algorithms?! ... i.e. can we simulate on a thimble?

Langevin is the natural candidate!

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

On the thimble by very definition! Noise should be extracted on the thimble!

But in our toy model we know very well the relevant direction: only 1 dimension, and thus the tangent space amounts simply to the only direction you always know, i.e. that of the gradient of the action!
Algorithms?! A generalization of Langevin

Langevin is the natural candidate!

\[
\frac{d}{d\tau} \phi^{(R)}_{a,x} = -\frac{\delta S_R}{\delta \phi_{a,x}} + \eta^{(R)}_{a,x} \\
\frac{d}{d\tau} \phi^{(I)}_{a,x} = -\frac{\delta S_R}{\delta \phi_{a,x}} + \eta^{(I)}_{a,x}
\]

On the thimble by very definition! Noise should be tangent to the thimble!

But since at the critical point we know the tangent space, the problem is that of transporting a vector along our gradient flow

\[\mathcal{L}_{\partial S_R}(\eta) = 0 \quad \Leftrightarrow [\partial S_R, \eta] = 0\]
Algorithms?! How accurate must one be with Langevin?

In principle everything is there, in particular

\[ \mathcal{L}_{\partial S_R}(\eta) = 0 \quad \iff \quad [\partial S_R, \eta] = 0 \]

\[ 0 = [\partial S_R, \eta(\tau)]_k = \sum_j \partial_j S_R \partial_j \eta_k(\tau) - \sum_j \eta_j(\tau) \partial_j \partial_k S_R \]

\[ \iff \quad \frac{d}{dT} \eta_j(\tau) = \sum_k \eta_k(\tau) \partial_k \partial_j S_R, \]

A question relevant in practice is: how much shall we go down towards the critical point?

Region of applicability of the

Hessian computed in \( \phi_{\min} \)

Here we evolve with Langevin
Algorithms?! A very crude approach ...

Region of applicability of the Hessian computed in $\phi_{\text{min}}$

1. The homology class of the thimble should be preserved (when this is not the case, the system will diverge).
2. The fluctuations in $S_I$ should be limited, to keep the sign problem away.

Here we evolve with Langevin

Applying the Algorithm

In principle everything there, in particular

Crudest approximation of the thimble 

i.e. the flat vector space associated to positive eigenvalues of the Hessian:

Equivalently:

how long needs the 5th dimension be?

Region of applicability of the Hessian computed in $\phi_{\text{min}}$
There are cases in which it works!

The Bose gas on the thimble
(Cristoforetti, Di Renzo, Mukherjee, Scorzato Phys. Rev. D 88 2013)
There are cases in which it works!

\[
\phi_{\text{min}} \quad \phi (s = \tau = 0)
\]

The Bose gas on the thimble
(Cristoforetti, Di Renzo, Mukherjee, Scorzato Phys. Rev. D 88 2013)
And there are cases in which it does not work!

A tribute to Kim’s CRM model!
Yet another algorithm: Metropolis

Originally proposed for U1 one-plaquette model (Cristoforetti, Mukherjee, Scorzato PRD Rapid 88 2013)

\[ S[\phi] = S[\phi_0] + S_G[\eta] + \mathcal{O}(|\eta|^3) \]

\[ S_G = \frac{1}{2} \sum_k \lambda_k \eta_k^2 \]

The idea of a Metropolis stems from the fact that near the critical point the action is gaussian and so ...

- Consider the theory that is purely gaussian and in the proximity of the critical point it approximates well the complete theory

- Extract a point for that theory and ...

- ... take a SD towards the critical point down to the region where the two theories are equivalent and ...

- ... take a SA from that point for the complete theory

- Accept/reject with

\[ P_{\text{acc}} = \min \left\{ 1, e^{-[S_R(\phi')-S_R(\phi)]+[S_G(\eta')-S_G(\eta)]} \right\} \]
Yet another algorithm: Metropolis

It works very well for our toy model (the algorithm has a technical parameter on which it depends!)
Yet another algorithm: ...

Notice that for a 0-dim toy model an algorithm can be implemented that performs ideal sampling.

The idea is simple: on each SD curve there is a 1-1 correspondence configuration-action, i.e. on a single SD if you extract a value for the action you extract a configuration ...

Leaving out a phase that is anyway corrected for (see immediately later!) ...

\[ Z_i = \int d z \ e^{-S_R(x,y)} \quad \rightarrow \quad Z_i = \int_{S_{P\sigma}}^\infty dS \ e^{-S_R} \left| \nabla S_R(t_S) \right|^{-1} \]

... but then we can invert

\[ F(S') = Z_i^{-1} \int_{S_{P\sigma}}^{S'} dS \ e^{-S_R} \left| \nabla S_R(t_S) \right|^{-1} \]

... extract a random number and get an action via

\[ F^{-1}(\xi) \]
The RESIDUAL PHASE

\[ \frac{1}{Z_0} \int_{\mathcal{J}_0} \prod_x d\phi_x e^{-S_R[\phi]} \mathcal{O}[\phi] \]

\[ \det(T_\phi) \]

(T_\phi \text{ is the tangent space to } \mathcal{J}_0 \text{ in } \phi.)

There is a residual phase, i.e. the Jacobian you would expect.

Good messages:

- Computed accurately in Fujii et al JHEP 1310 2013 and found tiny!

- Computable quite effectively via noisy estimators (last work of the thimble group: arXiv 1403.5637, accepted on PRD)
Conclusions

- A new regularization of field theories is getting more and more solid, legitimate and hopefully better and better computable.

- A few examples worked out quite nicely

- There is a lot of work to do. We were happy to see that someone else was working on the same subject (the Japanese group)! We hope in the near future other people could got involved as well.