Sign Problem and Lefschetz Thimbles

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Physical quantities of interest in QCD

- Just like in Stat Mech, our quantities of interest are the partition function Z and the expectation values-

$$\langle O(\phi) \rangle = \frac{\int \mathcal{D}\phi \; O[\phi] \; e^{-S[\phi]}}{\int \mathcal{D}\phi \; e^{-S[\phi]}} = \frac{1}{Z} \int \mathcal{D}\phi \; O[\phi] \; e^{-S[\phi]}.$$

- Discretize spacetime $\longrightarrow$ Evaluate integrals numerically.

Stat Mech.

βH

QFT

$S[\phi]$

Sign Problem

- Most common numerical method → Monte-Carlo Importance Sampling.

$$\langle O(\phi)\rangle = \frac{\int \mathcal{D}\phi\, O[\phi]\, e^{-S[\phi]}}{\int \mathcal{D}\phi\, e^{-S[\phi]}} = \frac{1}{Z}\int \mathcal{D}\phi\, O[\phi]\, \underbrace{e^{-S[\phi]}}_{\text{probability weight}}.$$

- $S[\phi] \in \mathbb{R} \implies e^{-S[\phi]} > 0$ → good prob. weight!

- But if $S[\phi] \in \mathbb{C} \implies e^{-S[\phi]} \in \mathbb{C}$ and is highly oscillatory. $\not> 0$

- In lattice field theory, the problem is also known as the **complex action problem** (NP-hard).

for 0-D models.

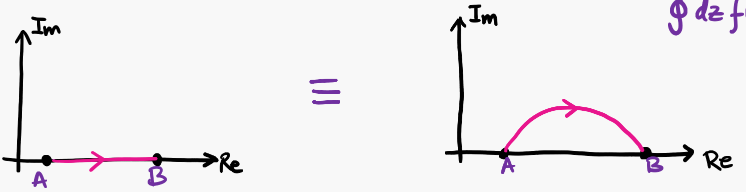
$$\langle O \rangle = \int_{-\infty}^{\infty} d\phi \, O(\phi) \frac{e^{-S(\phi)}}{Z}$$

General Problem: We want to calculate the following integral where $\rho(z)$ is a complex function

$$I(\lambda) = \int_{-\infty}^{+\infty} \mathrm{d}\phi \, f(\phi) \, e^{\lambda \rho(\phi)} \qquad \text{where } \phi \in \mathbb{R}.$$

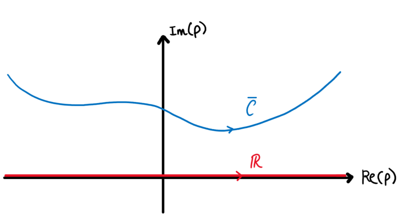
Possible Solution: Complexify $\phi \to z \in \mathbb{C} \longrightarrow$ use Cauchy's theorem (assuming $\rho(z)$ is analytic) and find a contour $\bar{\mathcal{C}}$ on which the integral is easier to evaluate.

$$\oint dz \, f(z) = 0$$



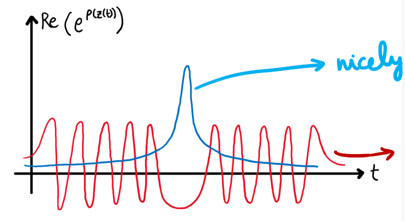
f(z) must be analytic in the r.o.i.

Lefschetz Thimbles (contd.)



All pts. meet at ∞ for contours extending over $\mathbb{C}$.

(a) Deformation of integration contours.



nicely peaked :)

highly oscillatory ö

(b) Integrand $\mathrm{Re}(e^{\rho})$ on $\mathbb{R}$ and $\bar{\mathcal{C}}$.

Figure: The effect of change of integration cycles.

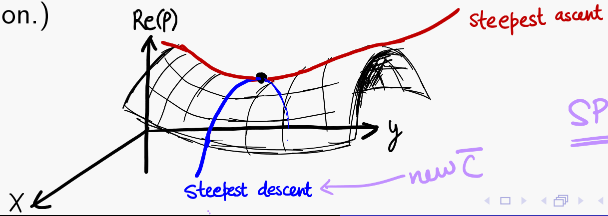
If such a $\bar{\mathcal{C}}$ exists, what does "easier to evaluate" mean?

- $\operatorname{Im}\rho$ is constant along $\bar{\mathcal{C}}$ (constant phase contour). → to kill ∿∿
- $\operatorname{Re}\rho$ decays away from the maximum at the fastest possible rate along $\bar{\mathcal{C}}$ (path of steepest-descent). → convergence.

One can show that-

Constant-phase contours $\equiv$ **Steepest contours**

These steepest descent and ascent contours always appear at the saddle point z_m of $\operatorname{Re}\rho$ i.e. $\rho'(z_m) = 0$. (since $\operatorname{Re}\rho$ is a harmonic function.)



SPM.

Lefschetz Thimbles (contd.)

$$\langle O(z) \rangle = \frac{\int \mathrm{d}z \, O(z) \, e^{-S(z)}}{\int \mathrm{d}z \, e^{-S(z)}}.$$

$\int dz \; f(z) \, e^{\rho(z)}$

Using this funda to find the steepest contours for our original problem, we will have $\rho(z) = -S(z)$.

- The critical points z_m are given by $S'(z_m) = 0$.
- The steepest contours are the same as the constant phase contours-

$z(t)$ parameter.

z_m $z(t)$ $t=0$

$$\operatorname{Im} S(z(t)) = \operatorname{Im} S(z_m) \xrightarrow[\text{w.r.t. } t]{\text{taking the derivative}} \frac{\mathrm{d}z(t)}{\mathrm{d}t} = -\overline{\frac{\mathrm{d}S}{\mathrm{d}z}\bigg|_{z(t)}}.$$

integrate backwards in time $t < 0 \longrightarrow$ steepest-descent contour (thimbles $\mathcal{J}_m$)
integrate forwards in time $t > 0 \longrightarrow$ steepest-ascent contours (anti-thimbles $\mathcal{K}_m$)

Lefschetz Thimbles (contd.)

Integrate $\dot{z} = -\overline{\partial_z S}$ "near" z_m

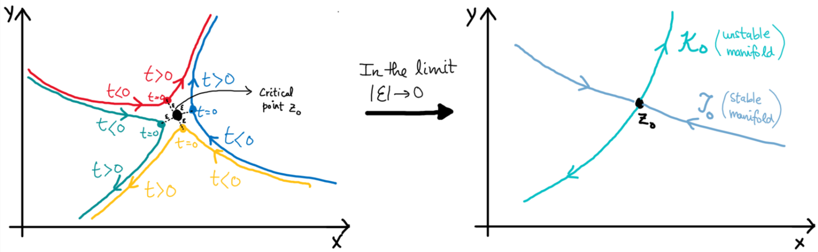
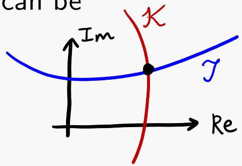


Figure: For numerical methods, we generally choose initial conditions very close to z_m, but in the limit $\epsilon \to 0$, a combination of all the trajectories gives the entire thimble/anti-thimble structure.

Need a way to relate original contour $\mathbb{R}$ to thimbles $\mathcal{J}_m$.

Lefschetz Thimbles (contd.)

Witten proved that the original integration contour can be decomposed into a sum over thimbles-



$$\int_{\mathbb{R}} = \sum_m \underbrace{\langle \mathcal{K}_m, \mathbb{R} \rangle}_{\text{weight}} \int_{\mathcal{J}_m}$$

$\langle \mathcal{K}_m, \mathbb{R} \rangle = c_m \longrightarrow$ no. of intersections the $\mathcal{K}_m$ makes with the $\mathbb{R}$.

Therefore, the expectation value integral can be decomposed as-

$$\int_{-\infty}^{\infty} dz \, \frac{O}{Z} e^{-S} \longrightarrow \langle O(z) \rangle = \frac{1}{Z} \sum_m c_m e^{-i \operatorname{Im} S(z_m)} \int_{\mathcal{J}_m} \mathrm{d}z \; e^{-\operatorname{Re} S(z)} O(z),$$

where the partition function Z is given by

$$\int_{-\infty}^{\infty} dz \, e^{-S} \longrightarrow \quad Z = \sum_m c_m e^{-i \operatorname{Im} S(z_m)} \int_{\mathcal{J}_m} \mathrm{d}z \; e^{-\operatorname{Re} S(z)}.$$

Quartic Model with a Linear Term

$$S(z) = \frac{\sigma}{2} z^2 + \frac{1}{4} z^4 + hz.$$

with $h = 1 + i$ and $\sigma = 1$. The critical points are found by solving for $\partial_z S = 0$

$$z^3 + z + (1 + i) = 0.$$

$z_0 = -0.799 - i0.359$
$z_1 = +0.219 + i1.369$
$z_2 = +0.580 - i1.01$

The Lefschetz flow equation for the model is-

$$\dot{x} = x^3 - 3xy^2 + x + 1, \qquad \dot{y} = y^3 - 3x^2 y - y - 1.$$

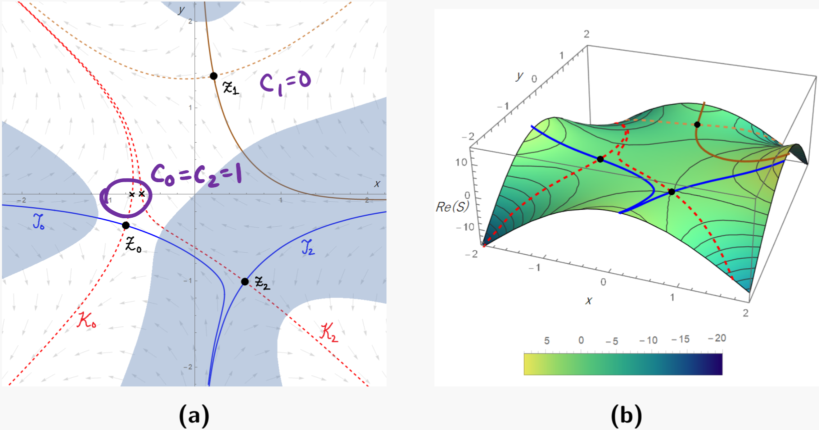


Figure: (a) thimble structure on the $\mathbb{C}$ plane. **(b)** the thimble structure on the manifold of Re(S).

Quartic Model with linear term (contd.)

The integral over $\mathbb{R}$ can be decomposed in this case as-

$$\int_{\mathbb{R}} = 1 \cdot \int_{\mathcal{J}_0} + \, 0 \cdot \int_{\mathcal{J}_2} + \, 1 \cdot \int_{\mathcal{J}_3}$$

Only the thimbles $\mathcal{J}_0$ and $\mathcal{J}_2$ contribute to the integral.

The partition function integral becomes-

$$Z = e^{-i \operatorname{Im} S(z_0)} \int_{\mathcal{J}_0} \mathrm{d}z \, e^{-\operatorname{Re} S(z)} \; + \; e^{-i \operatorname{Im} S(z_2)} \int_{\mathcal{J}_2} \mathrm{d}z \, e^{-\operatorname{Re} S(z)}.$$

Similar expression for $\langle O(z) \rangle$.

Evaluation of Z and $\langle O \rangle$

The results of numerical analysis of the thimble contour integrals gives the following results-

Obs.	Exact Value	from Lefschetz Thimble approach
Z	$1.76537 + i0.88721$	$1.75006 + i0.90277$
$\langle z \rangle$	$-0.49404 - i0.41732$	$-0.50203 - i0.42559$
$\langle z^2 \rangle$	$0.50857 + i0.30071$	$0.50444 + i0.30630$

Table: Numerical analysis for the Quartic model

The aim of the community is to generalise these methods to higher dimensional field theories (all of our discussion involved 0-D QFT).

Summary

Sign Problem: Failure to interpret $\underbrace{e^{-S}}$ as a probability weight for MC-IS.

$e^{-S(\phi)} \in \mathbb{C}$

Lefschetz Thimbles: Find new contours of integration called $\mathcal{J}_m$, equivalent to the original domain, along which the imaginary part of the action is constant and, therefore, the integral is (mostly) real.

$$\int_{\mathcal{J}} dz = \int_{-\infty}^{\infty} dt \, \underbrace{J(t)}_{\in \mathbb{C}}$$

"residual sign problem"

$\downarrow$

milder.

Primary References

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More details can be found in the full project report here.

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If our spacetime M is 0-D, then our "field" is a map

$\phi : \{pt\} \longrightarrow \mathbb{R}$ ⇝ 0-D field ≡ real variable

For 3+1-D spacetime, $\phi : \mathbb{R} \times \mathbb{R}^3 \longrightarrow \mathbb{R}$ ⇝ field

$S[\phi] \longrightarrow S(\phi)$