Lefschetz thimbles and sign problem: first results in 0 and 4 dimensional field theories

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Introduction: dense systems

Nuclear matter

Heavy Ion Collisions
Introduction: dense systems

\[ Z = \int \mathcal{D}A \det[\mathcal{D} + m - \mu \gamma_0/2] e^{S_{YM}} \]

The sign problem

at finite chemical potential
the fermionic determinant is complex:
standard Monte Carlo methods fails

\[ \det M(\mu) = |\det M(\mu)| e^{i\theta} \]

Unfortunately we cannot simply neglect the phase of the determinant. Phase quenched theory can be very different from the real world

An example of that difference that we will treat later is

the Silver Blaze phenomenon
Introduction: Lefschetz thimble

We want to overcome sign problem for Lattice QCD
We must be extremely careful not destroying physics

[ Silver Blaze phenomenon ]
whatever machinery we use to solve the theory

Integration on a Lefschetz thimble

Before applying the idea to full QCD we choose to
start from something more manageable: we consider
here integration on Lefschetz thimbles for the case
of a simple 0-dim field theory and
the 4-dim scalar field with a quartic interaction
**Lefschetz thimble on a lattice**

**Saddle point integration**

the Airy function

\[
\text{Ai}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i \left( \frac{t^3}{3} + xt \right)} dt
\]

\[t \rightarrow t_R + i t_I\]

- Complexify the variable
- Stationary point
- Steepest descent for the real part of the exponent starting at the stationary point
- Imaginary part of the exponent is constant

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**Diagram:**

- **Re** \[e^{i \left( \frac{t^3}{3} + xt \right)}\]
Lefschetz thimble on a lattice

Saddle point integration

It is a classic and elementary tool that works extremely well for low dimensional oscillating integrals.

It is usually combined with an asymptotic expansion around the stationary point. However, the idea of deforming the path is independent of the series expansion.

A path where the phase is stationary and the important contributions are more localized is very attractive from the point of view of the sign problem.

What about a Monte Carlo integral along the curves of steepest descent
Lefschetz thimble on a lattice

Path integral and Morse theory

- Complexify the degrees of freedom

\[ \int_{\mathbb{R}^n} dx^n g(x)e^{f(x)} \quad \cdots z = x + iy \cdots \int_C dz^n g(z)e^{f(z)} \]

- Deform appropriately the original integration path (Morse theory)

\[ \int_C dz^n g(z)e^{f(z)} = \sum_{\sigma} n_{\sigma} \int_{L_{\sigma}} dz^n g(z)e^{f(z)} \]

\[ L_{\sigma} \text{ for each stationary point } p_{\sigma} \text{ the } L_{\sigma} (\text{thimble}) \text{ is the union of the paths of steepest descent that fall in } p_{\sigma} \text{ at } \infty \]

\[ C = \sum_{\sigma} n_{\sigma} L_{\sigma} \text{ the thimbles provide a basis of the relevant homology group, with integer coefficients} \]

Generalization of the one dimensional SD to n-dim problems is called Lefschetz thimble
Can we use the thimble basis to compute the path integral for a QFT?

\[
\langle \mathcal{O} \rangle = \frac{\int_C \prod_x d\phi_x e^{-S[\phi]} \mathcal{O}[\phi]}{\int_C \prod_x d\phi_x e^{-S[\phi]}}
\]

The action is a Morse function also in the presence of gauge symmetry → stationary points are isolated
Lefschetz thimble on a lattice

Lefschetz thimbles and QFT
choosing the stationary point

The study of the stationary points of the complexified theory is mandatory and has to be done on a case-by-case

- consider the stationary point with the lower value of the real part of the action and with $n_\sigma \neq 0$

- this should be the one giving the dominant contribution (being the other vanishing or exponentially suppressed)

- there can be a symmetry connecting this with the other critical points

- if we can define around that point a QFT with the same degrees of freedom, the same symmetries and symmetry representations and the same perturbative expansion

\[
\langle \mathcal{O} \rangle = \frac{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \prod_x d\phi_x e^{-S[\phi]} \mathcal{O}[\phi]}{\sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \prod_x d\phi_x e^{-S[\phi]}}
\]

\[
\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{J}_0} \prod_x d\phi_x e^{-S[\phi]} \mathcal{O}[\phi]}{\int_{\mathcal{J}_0} \prod_x d\phi_x e^{-S[\phi]}}
\]

by universality we can look at the formulation of the path integral around that critical point as an acceptable regularization of the considered QFT
**Lefschetz thimbles and QFT**

**the residual phase**

\[
\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{J}_0} \prod_x d\phi_x e^{-S[\phi]} \mathcal{O}[\phi]}{\int_{\mathcal{J}_0} \prod_x d\phi_x e^{-S[\phi]}}
\]

- There is an additional phase coming from the Jacobian of the transformation between the canonical complex basis and the tangent space to the thimble.

- **Does it lead to a sign problem?**

  No formal proof but ...

  - \( d\Phi = 1 \) at leading order and \( \langle d\Phi \rangle \ll 1 \) are strongly suppressed by \( e^{-S} \)
  
  - there is strong correlation between phase and weight (precisely the lack of such correlation is the origin of the sign problem)
  
  - In fact this residual phase is completely neglected in the saddle point method
Integration on a Lefschetz thimble
M. C., F. Di Renzo and L. Scorzato
PRD86, 074506 (2012)

Is it numerically applicable to QFT’s on a Lattice?

Before applying the idea to full QCD we choose to start from something more manageable: we consider here integration on the Lefschetz thimbles for the case of

→ a 0 dimensional field theory with U(1) symmetry

→ the four dimensional scalar field with a quartic interaction
### Lefschetz thimble: algorithm

#### Langevin

\[
\frac{d\phi_i^R(\tau)}{d\tau} = -\frac{\delta S^R(\phi(\tau))}{\delta \phi_i^R(\tau)} + \eta_i^R(\tau)
\]

\[
\frac{d\phi_i^I(\tau)}{d\tau} = -\frac{\delta S^R(\phi(\tau))}{\delta \phi_i^I(\tau)} + \eta_i^I(\tau)
\]

#### Metropolis

\[\eta \rightarrow \text{n-dim random vector living on the manifold defined by the eigenvectors of the Hessian computed at the critical point with positive eigenvalues}\]

\[|\eta| \rightarrow \text{distance along the thimble}\]

\[|\eta|/\delta r \rightarrow \text{number of steps along the steepest descent}\]

\[
\frac{d\phi_i(r)}{dr} = \frac{1}{r} \frac{\delta S}{\delta \phi_i(r)}
\]

\[\phi_i(n + 1) = \phi_i(n) + \delta r \frac{\delta S}{\delta \phi_i}\]

projection of the noise on the tangent space
**Lefschetz thimble: algorithm**

Gaussian thimble

Gaussian manifold: flat manifold defined by the directions of steepest descent at the critical point

$|\eta|/\delta r = N$ → number of steps along the steepest descent

- Decreasing $\delta r$ your manifold get closer and closer to the Lefschetz thimble
- If the action decreases fast away from the stationary point integrating on the Gaussian thimble can be sufficient
Can be seen as the limiting case of the more interesting three-dimensional XY model

One dimensional problem: the integration on the Lefschetz thimble can be plotted

\[
S = -i \frac{\beta}{2} (U + U^{-1}) = -i \beta \cos \phi
\]

\[
\langle e^{i\phi} \rangle = i \frac{J_1(\beta)}{J_0(\beta)}
\]

On the thimble

\[
\langle O(\phi) \rangle = \frac{\sum \sigma m_\sigma \int_{\mathcal{J}_\sigma} d\phi O(\phi)e^{-S(\phi)}}{\sum \sigma m_\sigma \int_{\mathcal{J}_\sigma} d\phi e^{-S(\phi)}}
\]

\[
S_R = -\beta \sin \phi_R \sinh \phi_I
\]

\[
S_I = -\beta \cos \phi_R \cosh \phi_I
\]

constant on the thimble
The stationary points are in (0,0) and (\pi,0) and the thimble can be computed also analytically.

Exact thimbles: have to pass from the critical point and the imaginary part of the action has to be constant.

\[ S_I(\tau) = -\beta \cos \phi_R(\tau) \cosh \phi_I(\tau) = S^\text{cp}_I \]
The stationary points are in (0,0) and (\pi,0) and the thimble can be computed also analytically. In order to perform the integration on the thimble we use a Metropolis algorithm.

**Gaussian manifold**

Increasing the accuracy in the integration of the steepest descent we move closer to the exact thimble.

**U(1) one plaquette model**

U(1) one plaquette model


OBSERVABLE

\[ \langle e^{i\phi} \rangle = i \frac{J_1(\beta)}{J_0(\beta)} \]

There are parameter regions where integration on the Gaussian manifold is sufficiently accurate.
Residual phase is well under control and is not a source of additional sign problem (at least in this case).

\[
\langle \mathcal{O}(\phi) \rangle = \frac{\sum_{\sigma} m_{\sigma} \int_{\mathcal{J}_\sigma} d\phi \mathcal{O}(\phi) e^{-S(\phi)}}{\sum_{\sigma} m_{\sigma} \int_{\mathcal{J}_\sigma} d\phi e^{-S(\phi)}}
\]

There is an additional phase coming from the Jacobian of the transformation between the canonical complex basis and the tangent space to the thimble.

This phase should be essentially constant over the portion of phase space which dominates the integral.

\[
\cos(\arg \{ J_\eta^\phi e^{-S} \})
\]

Residual phase

Probability measure

Log scale
**Silver Blaze problem**
when $T=0$ and $\mu<\mu_c$ physics is independent from the chemical potential

We will study the system at zero temperature
\[ S[\phi, \phi^*] = \int d^4x (|\partial_\nu \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \lambda|\phi|^4 + \mu(\phi^* \partial_0 \phi - \partial_0 \phi^* \phi) \]

Continuum action

\[ S[\phi, \phi^*] = \sum_x [(2d + m^2)\phi^*_x \phi_x + \lambda(\phi^*_x \phi_x)^2 - \sum_{\nu=0}^4 (\phi^*_x e^{-\mu\delta_{\nu,0}} \phi_{x+\hat{\nu}} + \phi^*_{x+\hat{\nu}} e^{\mu\delta_{\nu,0}} \phi_x)] \]

Lattice action: chemical potential introduced as an imaginary constant vector potential in the temporal direction

in term of real fields \( \phi_a (a = 1, 2) \)

\[ \phi = \frac{1}{\sqrt{2}} (\phi_1 + i\phi_2) \]

\[ S[\phi_a] = \sum_x \left[ \frac{1}{2} (2d + m^2)\phi^2_{a,x} + \frac{\lambda}{4} (\phi^2_{a,x})^2 - \sum_{\nu=1}^3 \phi_{a,x} \phi_{a,x+\hat{\nu}} \right] \]

\[ = \cosh \mu \phi_{a,x} \phi_{a,x+\hat{0}} + i \sinh \mu \varepsilon_{ab} \phi_{a,x} \phi_{b,x+\hat{0}} \]
\[ S[\phi, \phi^*] = \int d^4x (|\partial_\nu \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \lambda|\phi|^4 + \mu(\phi^* \partial_0 \phi - \partial_0 \phi^* \phi) \]

\[ \langle O \rangle_{\text{full}} = \frac{\int \mathcal{D}\phi |e^{-S}| e^{i\theta} \mathcal{O}}{\int \mathcal{D}\phi |e^{-S}| e^{i\theta}} = \frac{\langle e^{i\theta} \mathcal{O} \rangle_{pq}}{\langle e^{i\theta} \rangle_{pq}} \]

Let us try ignoring the phase

\[ \langle O \rangle_{pq} = \frac{\int \mathcal{D}\phi |e^{-S}| \mathcal{O}}{\int \mathcal{D}\phi |e^{-S}|} \]
$S[\phi, \phi^*] = \int d^4x (|\partial_\nu \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \lambda|\phi|^4 + \mu(\phi^* \partial_0 \phi - \partial_0 \phi^* \phi)$

\[ \langle n \rangle = \frac{1}{V} \frac{\partial \ln Z}{\partial \mu} \]
On the Lefschetz thimble
M. C., F. Di Renzo, A. Mukherjee and L. Scorzato

☐ Fields are complexified \( \phi_a \rightarrow \phi_a^R + i\phi_a^I \)

☐ The integration on the thimble performed with a Langevin algorithm

☐ In this case calculations in Gaussian approximation are sufficient to obtain the exact result
$\lambda \Phi^4$ on a Lefschetz thimble

On the Lefschetz thimble
M. C., F. Di Renzo, A. Mukherjee and L. Scorzato

Silver Blaze
solving sign problem we have the correct physics
$\lambda \Phi^4$ on a Lefschetz thimble

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Comparison with Worm Algorithm
(courtesy of C. Gattringer and T. Kloiber)

\[
\langle n \rangle = \frac{1}{V} \frac{\partial \ln Z}{\partial \mu}
\]
Something else on a Lefschetz thimble

Next steps

- XY Model
- Hubbard model (involves a determinant)
- ...
- move to QCD
thank you