Sign Problem and Lefschetz Thimbles

Kunal Verma and Anosh Joseph
Department of Physical Sciences, Indian Institute of Science Education and Research - Mohali, Knowledge City, Sector 81, SAS Nagar, Punjab 140306, India
(Dated: December 4, 2022)

Sign Problem in the quantum Monte Carlo (QMC) method is prevalent across quantum many-body simulations. Recent work has led to the development of several candidate methods to deal with the sign problem. In this article, we will present a pedagogical overview of the progress to cure this problem by one of the potential candidates, known as the Lefschetz thimble method. The method relies on complexifying the field variables, and calculating the integral over a new equivalent manifold along which the imaginary part of the action is constant and the integral is (mostly) real.

I. INTRODUCTION

Quantum Monte Carlo (QMC) method is a potent tool to study quantum many-body lattice models in physics numerically. The method casts the partition function of the theory as a sum (or an integral) over all the configurations, converts it to a classical sum (in some particular limit), and then evaluates the sum using importance sampling techniques to cherry pick the "relevant" regions of the configuration space C. The partition function Z has the form

$$Z = \mathrm{Tr}(\hat{\rho}) = \sum_i \langle \phi_i | \hat{\rho} | \phi_i \rangle \approx \sum_C \rho(C).$$

The term $\rho(C)$ is interpreted as a probability weight. (For thermal systems, the partition function can be traced over the energy eigenstates, resulting in $\rho(C) = e^{-\beta E(C)}$, the familiar Boltzmann weight.) Instead of summing over all the possible configurations, a Markov Chain constructed with an equilibrium distribution $\rho(C)$ samples over the most relevant configurations in the space (once it has equilibrated). These relevant configurations can be used to compute expectation values of operators $\langle O \rangle$.

However, this method has a severe shortcoming. Suppose the weight $\rho(C)$ is negative or even complex. In that case, it can no longer be interpreted as a *probability* weight, leading to the infamous *sign problem* (which is an NP-hard problem).

In the context of quantum many-body problems, the weight $\rho(C) \sim e^{-S[\phi]}$, where $S[\phi] \in C$, when the fermions have a nonzero chemical potential $\mu \neq 0$. The first line of attack towards such problems is to *reweight* the weight by decomposing it into its modulus and phase. However, the resulting Monte Carlo averages in the numerator and denominator (when computing expectation values) are so small that they get swamped by the inherent noise in MC sampling and converge to incorrect results.

As an attempt to "cure" this sign problem, several techniques have been proposed with partial success, but the sign problem is still unsolved for several significant physics problems. One of the recently proposed candidates, which we will review in this article, is known as the *Lefschetz thimbles method.*

In this article, we will only consider $0+0$-dimensional lattice models. Let us say we map the quantum problem onto a classical problem via certain transformations, which is a regular exercise for many-body physicists, then the expectation value of an observable O is defined as the following integral over all field configurations

$$\langle O \rangle = \frac{\int D\phi \, O(\phi) \, e^{-S(\phi)}}{\int D\phi \, e^{-S(\phi)}} = \frac{1}{Z} \int D\phi \, O(\phi) \, e^{-S(\phi)}. \quad (1)$$

If the integral is plagued with the "sign problem", then the weight, $e^{-S(\phi)}$ is expected to be *highly oscillatory.* We need incredibly high precision to calculate such integrals using the standard numerical integration, and it can be impractical. We discuss in the following section a way to get around this.

II. DEFORMING THE INTEGRATION CONTOUR

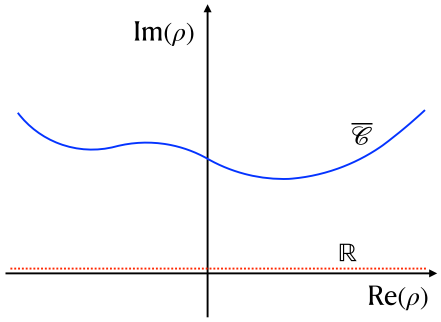
Let us start with a generic integral where our integrand is highly oscillatory

$$I(\lambda) = \int_{-\infty}^{+\infty} d\phi \, f(\phi) \, e^{\lambda \rho(\phi)}, \quad (2)$$

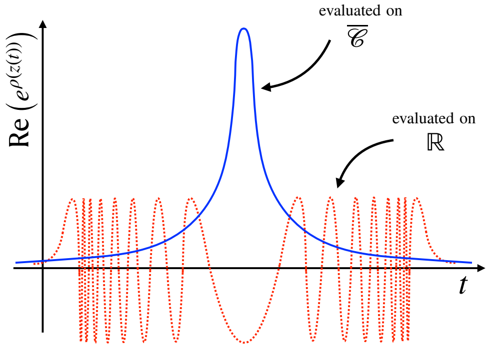
where λ is a parameter, $\phi \in \mathbb{R}$, and $f(\phi)$ and $\rho(\phi)$ are functions of ϕ.

Here we assume that $\rho(\phi) : \mathbb{R} \to \mathbb{C}$, thereby creating rapid oscillations, making ordinary numerical integration hopeless. To fix this, we can think of the problem in an equivalent but powerful way, i.e., we can think of the above integral as a *contour integral over* $\overline{\mathcal{C}}$ *in the complex plane.*

There is an advantage for complexifying the variable $\phi \to z \in \mathbb{C}$. We can now use *Cauchy's integral theorem* to deform the integration contour in the domain of analyticity. Suppose we can find a contour along which $\mathrm{Im}(\rho(z)) =$ constant, then the oscillations of the integrand can be suppressed. We can safely perform numerical integration of the function along these contours. Fig. 1 shows a pictorial representation of the same.



(a) Deformation of integration contours.



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

FIG. 1: The effect of change of integration cycles. (a) The integration contour $\mathbb{R}$ (dashed curve in red color) is deformed into a contour $\overline{\mathcal{C}}$ (solid curve in blue color). Both the contours meet at infinity, respecting Cauchy's theorem. (b) The rapid oscillations of the integrand almost disappear if the integrand $\mathrm{Re}(e^{\rho})$ is evaluated along the contour $\overline{\mathcal{C}}$.

A. Do Such Special Contours Exist?

As shown in Fig. 1, we desire to deform the original integration path to a *special contour*, $\overline{\mathcal{C}}$, on which the integral is easier to evaluate. What does "easier to evaluate" mean in the context of our problem?

1. $\mathrm{Im}(\rho(z))$ = constant along the special contour $\overline{\mathcal{C}}$ (constant phase contour).
2. $\mathrm{Re}(\rho(z))$ decays away from the maximum at the fastest possible rate along $\overline{\mathcal{C}}$ (path of steepest descent).

Now, as it turns out, the magic of *complex analysis* does most of the work for us, and one can show with a few lines of calculations that:

$$\textit{Constant phase contours} \equiv \textit{Steepest contours}$$

This remarkable result provides us with the path of steepest descent (or ascent) for free once we find the constant phase contour.

B. Saddle Point Method

It is now natural to argue using elementary complex analysis that the steepest descent and ascent contours (which are also constant phase contours) arise at the *saddle point* of the function $\rho(z)$ since $\mathrm{Re}(\rho)$ and $\mathrm{Im}(\rho)$ are harmonic functions. The saddle points z_m of a function are defined to be the points where

$$\rho'(z_m) = 0,$$

with the prime denoting differentiation with respect to z. Therefore, our strategy to move forward is as follows. The constant phase contours $\mathrm{Im}(\rho)$ = constant, emanating from the saddle points z_m of $\rho(z)$, generate the steepest descent (and ascent) contours. We desire to integrate our function over this steepest descent contour, which we will refer to as the *Lefschetz thimble*. The corresponding steepest ascent contour is the *Lefschetz anti-thimble*.

III. FINDING THE LEFSCHETZ THIMBLES (AND ANTI-THIMBLES)

For our specific problem of calculating the partition function and expectation values, we can use the concepts developed in the last section with a few identifications.

From Eq. (1), we identify $\rho(z) = -S(z)$. We proceed as follows

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

  $$\mathrm{Im}(S(z(t))) = \mathrm{Im}(S(z_m)),$$

  since the contours must go through the saddle points z_m.

If we take the derivative with respect to t (which parameterizes the contour) in the constant phase condition, we generate the *flow equation* of the system

$$\begin{aligned} S(z(t)) - \overline{S(z(t))} &= \text{const.} \\ \implies \frac{dS}{dz}\bigg|_{z(t)} \frac{dz}{dt} - \overline{\frac{dS}{dz}}\bigg|_{z(t)} \overline{\frac{dz}{dt}} &= 0. \end{aligned} \tag{3}$$

The bar ($\overline{S}$) here denotes complex conjugation. One of the possible flow equations that satisfy the above condition is

$$\frac{dz(t)}{dt} = -\overline{\frac{dS}{dz}}\bigg|_{z(t)}. \tag{4}$$

The above flow equation is known as the *Lefschetz flow equation* and is one of the possible flow equations to generate the contours. The general procedure to generate

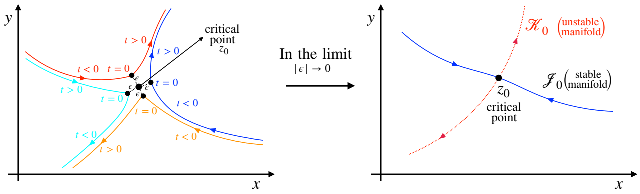


FIG. 2: Combining the curves generated from integrating the flow equation from two or more ϵ-neighbourhood points of the saddle point z_0 gives the entire thimble/anti-thimble structure.

the contours is to integrate the flow equation (4) starting from the associated saddle point $z(t=0) = z_m$. It can also be verified by separating the flow equation into real and imaginary parts and linearizing the system around the critical points z_m that the eigenvalues of the flow are given by

$$\lambda_{1,2} = \pm \left| \vec{\nabla} \mathrm{Re} S'(z) \right|, \tag{5}$$

thus verifying that the critical points are indeed saddle points.

We also make the following interesting observation

$$\begin{aligned} \frac{d}{dt}\mathrm{Re}(-S) &= -\frac{1}{2}\frac{d}{dt}(S+\overline{S}) \\ &= -\frac{1}{2}\left(\frac{dS}{dz}\frac{dz}{dt} + \overline{\frac{dS}{dz}}\,\overline{\frac{dz}{dt}}\right) \\ &= = + \left|\frac{dS}{dz}\right|^2 \geq 0. \end{aligned} \tag{6}$$

If we integrate the flow equation starting from $z(t=0) = z_m$ we find:

- Integrating backwards $t < 0$ generates a curve on which $\mathrm{Re}(-S)$ monotonically decreases. It is the steepest descent curve: the thimble $\mathcal{J}_m$.
- Integrating forwards $t > 0$ generates a curve on which $\mathrm{Re}(-S)$ monotonically increases. It is the steepest ascent curve: the anti-thimble $\mathcal{K}_m$.

In the language of dynamical systems, these curves are also known as stable and unstable manifolds, respectively.

However, when generating these curves numerically, one must be cautious. Since the saddle points, by definition, are "fixed points" that have vanishing flow, one has to integrate the flow equations from two or more ϵ-neighborhood points of the saddle point z_m to get the entire thimble/anti-thimble structure (see Fig. 2).

IV. THIMBLE DECOMPOSITION FORMULA

The important result which was proposed by Witten [2] states that we can replace the integration over the real domain $\mathbb{R}^n$ with that over the thimbles $\mathcal{J}_m$:

$$\begin{aligned} \int_{\mathbb{R}^n} & d^n\phi\, O(\phi)\, e^{-S(\phi)} \\ &= \sum_m \langle \mathcal{K}_m, \mathbb{R}^n \rangle \int_{\mathcal{J}_m} d^n z\, O(z)\, e^{-S(z)}. \end{aligned} \tag{7}$$

This expression gives us a simple recipe for deforming our original integration contour. The term

$$\langle \mathcal{K}_m, \mathbb{R}^n \rangle = c_m \tag{8}$$

are the *intersection numbers* of the anti-thimbles $\mathcal{K}_m$ with the original integration contour $\mathbb{R}^n$. For 0 + 0-dimensional lattice models, $\mathbb{R}^n$ is replaced with $\mathbb{R}$.

The expectation value integral can be decomposed as

$$\langle O(z) \rangle = \frac{1}{Z}\sum_m c_m e^{-i\mathrm{Im}S(z_m)} \int_{\mathcal{J}_m} dz\, e^{-\mathrm{Re}S(z)} O(z), \tag{9}$$

where the partition function Z is given by

$$Z = \sum_m c_m e^{-i\mathrm{Im}S(z_m)} \int_{\mathcal{J}_m} dz\, e^{-\mathrm{Re}S(z)}. \tag{10}$$

The above contour integrals along $\mathcal{J}_m$ can be calculated by appropriately parameterizing the thimbles, which also introduces the so-called *residual phase* (arising from the Jacobian due to the thimble curvature). For a thimble $\mathcal{J}_0$ with saddle point z_0, if we parameterize the thimble as follows:

$$\mathcal{J}_0 : \quad x(t) + iy(t), \quad -\infty < t < \infty, \tag{11}$$

it results in

$$\int_{\mathcal{J}_0} dz = \int_{-\infty}^{+\infty} dt\, J(t), \tag{12}$$

where $J(t)$ is the complex Jacobian $J(t) = x'(t) + iy'(t)$ that introduces the *residual sign problem.* Note that the residual sign problem is much milder than the initial sign problem we started with.

Therefore, together with the recipe for the thimble decomposition given in Eq. (7) and the methodology to generate thimbles and anti-thimbles, we are now ready to attack the sign problem with the entire machinery of the Lefschetz thimble method. We demonstrate this with a toy model example.

V. A TOY MODEL EXAMPLE: QUARTIC MODEL WITH A LINEAR TERM

To demonstrate the application of the Lefschetz thimble method, we explore the simplest example of a non-trivial zero-dimensional field theory with a linear source term. The action of this theory has the following form (after complexifying the fields from $\phi \to z \in \mathbb{C}$)

$$S(z) = \frac{\sigma}{2}z^2 + \frac{1}{4}z^4 + hz. \tag{13}$$

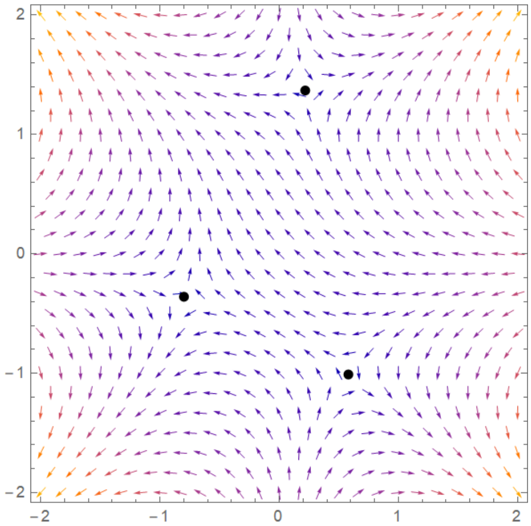


FIG. 3: Lefschetz flow for the quartic model.

We will use the specific parameters, $\sigma = 1$ and $h = 1 + i$.

The Lefschetz flow equation for this system is given by

$$\frac{dz}{dt} = -\overline{S'(z)} = -(\overline{z}^3 + \overline{z} + \overline{1+i}). \tag{14}$$

On separating the equation into real and imaginary parts, we get

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

As mentioned earlier, this system can be viewed as a two-dimensional dynamical system with a saddle point flow, as shown in Fig. 3. The saddle points can be found by solving for $S'(z) = 0$, i.e.,

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

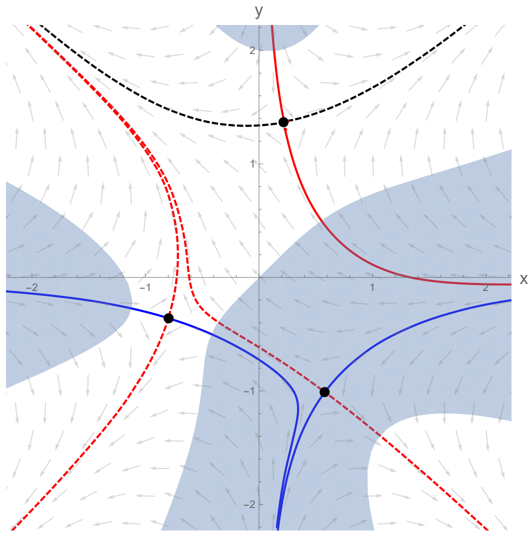
The solution gives the three saddle points as

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

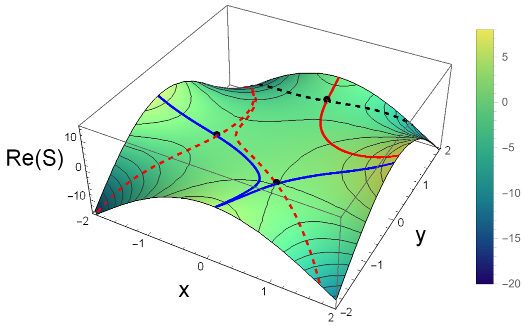
As discussed in the previous section, for each saddle point z_m, there exists a corresponding thimble $\mathcal{J}_m$ and an anti-thimble $\mathcal{K}_m$. We obtain each thimble (and anti-thimble) from the union of the curves obtained by integrating the flow equation around two ϵ-neighborhood points of z_m (see Fig. 4).

We see that the *contributing* thimbles $\mathcal{J}_m$ in Fig. 4a end in the region of convergence (the shaded region). This region is defined by $\mathrm{Re}(S) > 0$, which ensures that $S \to \infty$ sufficiently rapidly along a thimble, thus making the integral containing $\exp(-S)$ convergent.

We also see that the anti-thimble $\mathcal{K}_1$ corresponding to the saddle point z_1 does not intersect with the original integration domain $\mathbb{R}$. Since $c_1 = 0$, the thimble $\mathcal{J}_1$ does not contribute to the partition function and thus the expectation value. Both anti-thimbles $\mathcal{K}_0$ and $\mathcal{K}_2$ intersect exactly once with $\mathbb{R}$, so $c_{0,2} = 1$.



(a)



(b)

FIG. 4: Thimble structure with the Lefschetz flow for the quartic model. (a) The black circles represent the fixed points $z_{0,1,2}$ with solid lines (blue) indicating thimbles and dashed lines (red) anti-thimbles, which contribute to the integral Z. The red solid and black dashed pair of contours does not contribute since the anti-thimble does not intersect with the $\mathbb{R}$ line. (b) The thimble structure is shown on the manifold of $\mathrm{Re}(S)$. Since the thimbles $\mathcal{J}_m$ are defined as the steepest descent contours of $\mathrm{Re}(-S)$, they appear like the steepest ascent contours of $\mathrm{Re}(S)$ (and vice-versa for anti-thimbles $\mathcal{K}_m$).

A. Calculating the Integrals

With $c_1 = 0$ and $c_{0,2} = 1$, the partition function integral can be decomposed as

$$Z = e^{-i\mathrm{Im}S(z_0)} \int_{\mathcal{J}_0} dz\, e^{-\mathrm{Re}S(z)} + e^{-i\mathrm{Im}S(z_2)} \int_{\mathcal{J}_2} dz\, e^{-\mathrm{Re}S(z)}. \tag{15}$$

The expectation value of the observable is written similarly

$$\langle O(z)\rangle = \frac{1}{Z}\Big[e^{-i\mathrm{Im}S(z_0)}\int_{\mathcal{J}_0} dz\; e^{-\mathrm{Re}S(z)}O(z) + e^{-i\mathrm{Im}S(z_2)}\int_{\mathcal{J}_2} dz\, e^{-\mathrm{Re}S(z)}O(z)\Big]. \quad (16)$$

The real and imaginary parts of the action can be written as

$$\mathrm{Re}S = \frac{1}{4}(4x + x^4 + 2x^2(1-3y^2) + y(y^3 - 2y - 4)),$$
$$\mathrm{Im}S = y + x^3 y + x(1 + y - y^3),$$

and are to be substituted in the above expressions for Z and $\langle O(z)\rangle$.

It is also important to parameterize the thimbles $\mathcal{J}$ in a manner such that for the combination of thimbles, the composed direction of parameterization should roughly move from left to right, i.e., in the direction of going from $-\infty$ towards $+\infty$, to ensure a correct decomposition from the original integration contour $\mathbb{R}$.

Once we have a working setup, it is a simple exercise to numerically evaluate the above integrals using a standard numerical integration package. All the numerics in this article were performed using `RK4` numerical integration in `Mathematica`.

For demonstration purposes, we calculate the partition function Z and the expectation values of the first and second moments, i.e., $\langle z\rangle$ and $\langle z^2\rangle$, and compare them with the exact values. In Table I, we show the results we get by adding the contributions from numerical integration along the thimbles $\mathcal{J}_0$ and $\mathcal{J}_2$.

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 I: Numerical analysis for the quartic model.

VI. SUMMARY AND OUTLOOK

The method of Lefschetz thimbles is a powerful tool to study field theory systems that exhibit the sign problem. However, we note that the parameterized integrals along the thimbles still suffer from a residual sign problem, arising due to the Jacobian, $J(t)$ of the transformation of the field variables. In cases like the quartic model studied here, the residual phase is not rapidly oscillating, so numerically integrating the function using simple grid-based or Monte Carlo integration does not require high precision. There are models where the residual sign problem is not as mild, and active research is being carried out to reduce its severity.

Therefore, by no means is the Lefschetz thimble approach a complete solution to the sign problem. It might be impossible to find a general solution. However, it is a helpful approach in reducing the severity of the sign problem in various critical physical problems of interest.

Acknowledgements

An initial version of this article was prepared by KV as a summer project report [3] at IISER Mohali in 2021. AJ is partially supported by IISER Mohali. KV is partially supported by the INSPIRE Scholarship for Higher Education by the DST, Government of India.

Data Availability Statement

No Data associated in the manuscript.

[1] Y. Tanizaki, *Study on sign problem via Lefschetz-thimble path integral.* PhD Thesis, The University of Tokyo (2015), pp. 11-18 (PhD Thesis).
[2] E. Witten, *Analytic Continuation Of Chern-Simons Theory,* AMS/IP Stud. Adv. Math. **50** (2011), 347-446; pp. 10-14; arXiv:1001.2933 [hep-th].
[3] K. Verma, *Numerical Methods for Evading the Sign Problem: A Primer on Complex Langevin and Lefschetz Thimble Methods*, Summer Project Report (2021) (Project Report).
[4] L. Bongiovanni, *Numerical Methods for the Sign Problem in Lattice Field Theory,* PhD Thesis (2016); arXiv:1603.06458 [hep-lat].
[5] R. Bharathkumar and A. Joseph, *Lefschetz Thimbles and Quantum Phases in Zero-Dimensional Bosonic Models,* Eur. Phys. J. C **80**, no.10, 923 (2020) arXiv:2001.10486 [hep-th].
[6] G. Pan, Z. Y. Meng, *Sign Problem in Quantum Monte Carlo Simulation*, Book chapter for Elsevier Encyclopedia of Condensed Matter Physics, arXiv:2204.08777 [cond-mat.str-el].
[7] Steven H. Strogatz, *Nonlinear dynamics and Chaos: With Applications to Physics, Biology, Chemistry, and Engineering*, CRC Press (2019), pp. 125-145.
[8] C. M. Bender, S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers I: Asymptotic Methods and Perturbation Theory*, Springer New York, (1999), pp. 247-306.