On a modification method of Lefschetz thimbles

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Reference: S. T., and Takahiro M. Doi, PRD94, 074009 (2016)

Sign problem

Monte-Carlo (MC) integration:
a very efficient way of numerical integration

$$\int dx O(x) P(x) \sim \frac{1}{N} \sum_{i=1}^{N} O(x_i)$$

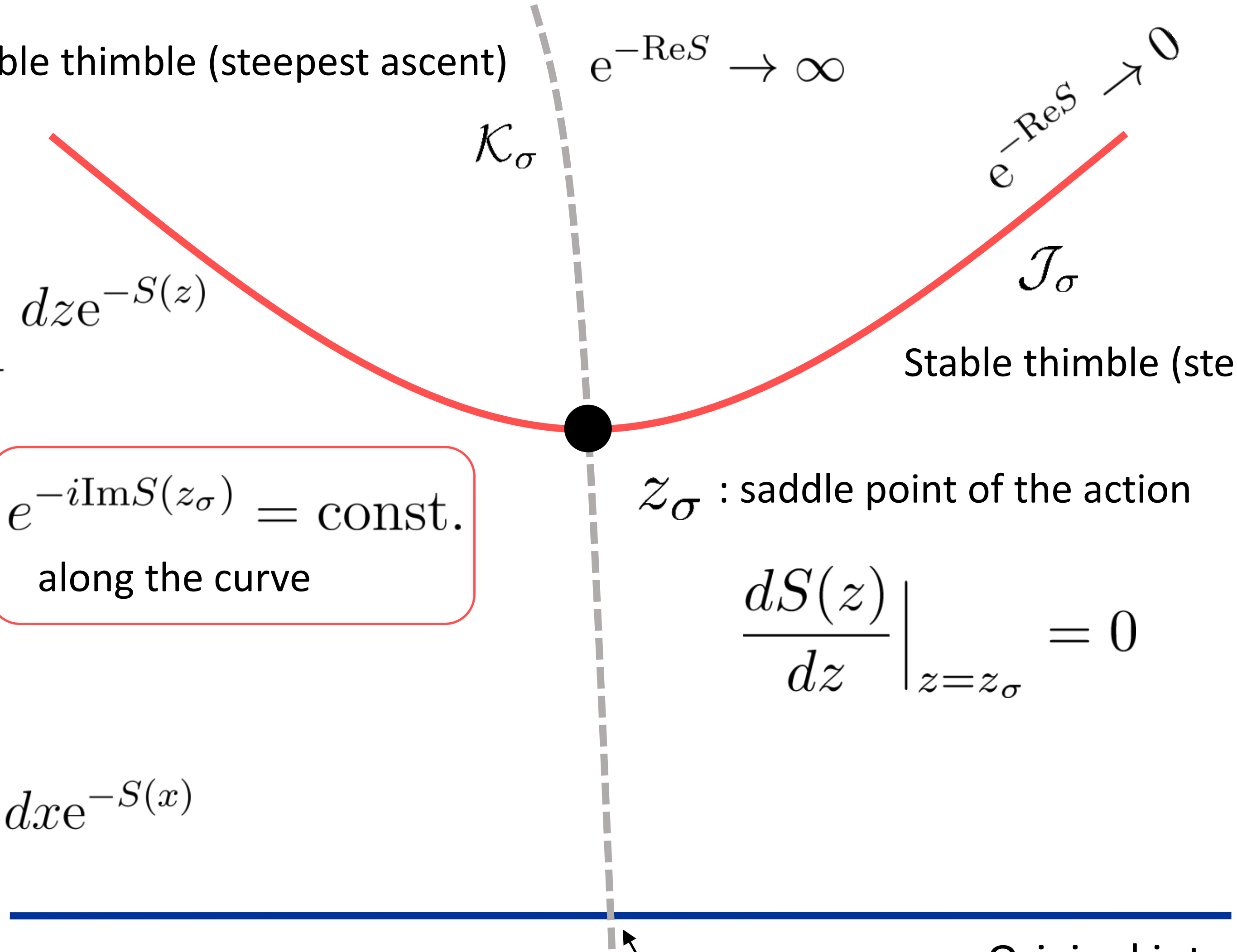
x_i is a random variable with the distribution $P(x)$

However, in many (interesting) cases, $S(x) \in \mathbb{C}$

$$Z = \int dx e^{-S(x)}$$

the Boltzmann factor is no longer
a probability distribution

Lefschetz thimble



$$Z = \int_{\mathcal{J}_\sigma} dz e^{-S(z)}$$

$$e^{-i\mathrm{Im}S(z_\sigma)} = \mathrm{const.}$$

along the curve

$$\left.\frac{dS(z)}{dz}\right|_{z=z_\sigma} = 0$$

$$Z = \int dx e^{-S(x)}$$

Thimble decomposition

Pham (1983), Witten (2001)

$$Z = \int dx e^{-S(x)} = \sum_{\sigma=1}^{N_{\mathrm{sp}}} n_\sigma e^{-i\mathrm{Im}S(z_\sigma)} \int_{\mathcal{J}_\sigma} dz e^{-\mathrm{Re}S(z)}$$

Original partition fnc.

Decomposition to Lefschetz thimbles

z_σ : saddle point of the action

N_{sp} : Number of saddle points

$$\left.\frac{dS(z)}{dz}\right|_{z=z_\sigma} = 0$$

$\mathcal{K}_\sigma$: Unstable thimble (steepest ascent)

$\mathcal{J}_\sigma$: Stable thimble (steepest descent)

n_σ : intersection number of the original integration path and unstable thimble

Basically, $n_\sigma = 0, 1$

Motivation

Question 1: How many relevant thimbles are there?

- Away from phase transition lines, the number of thimbles tends to be one. Indeed, single-thimble approximation works well in some cases.
- Near the transition lines, one should pick up more than one thimble. (In field theories, this task may be harder.)

Question 2: Why integration on multi-thimbles is difficult?

- It is difficult to collect all relevant saddle points.

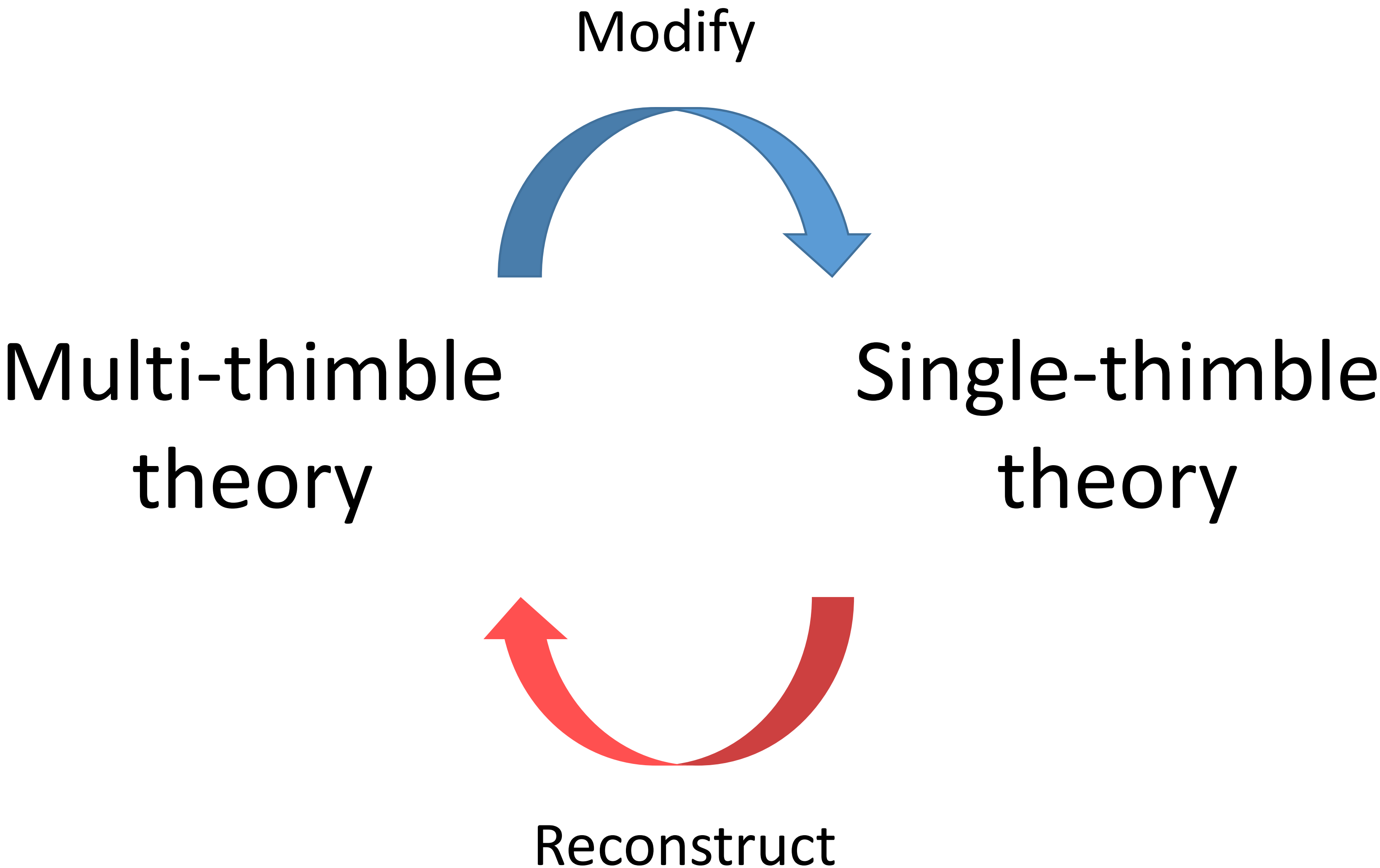
  Holomorphic gradient flow — Alexandru, Basar, Bedaque, Ridgway, Warrington (2016); Tanizaki, Nishimura, Verbaarschot (2017)

- Usual Monte-Carlo technique does not work.

  Parallel tempering — Alexandru, Basar, Bedaque, Warrington (2017); Fukuma, Umeda (2017)

- Global sign problem can be severe.

Our strategy

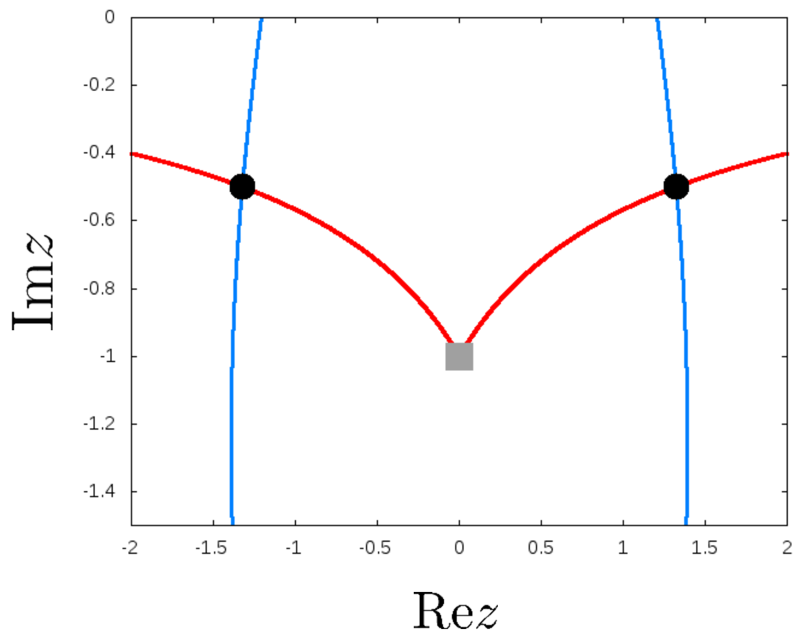


A toy model

$$Z = \int dx\ (x + i\alpha)^2 \mathrm{e}^{-x^2/2} \qquad (\alpha \in \mathbb{R})$$

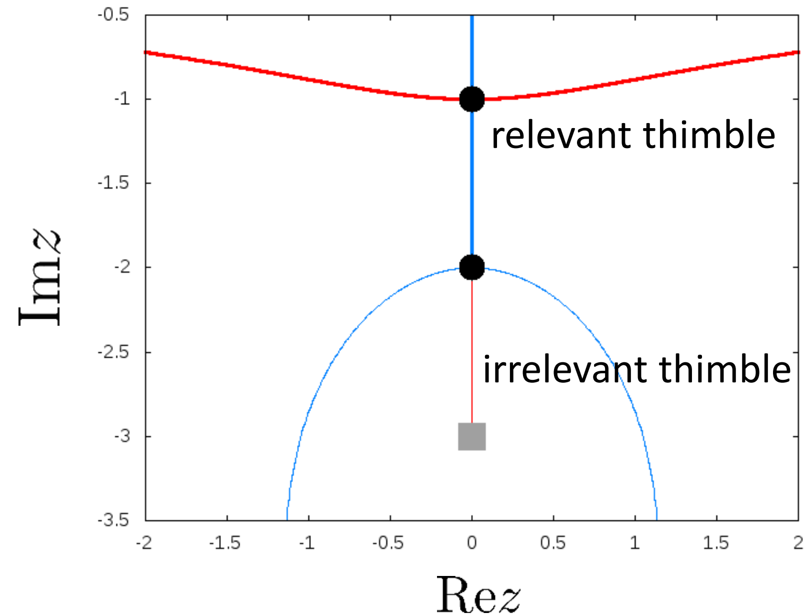
Cf) J. Nishimura, S. Shimasaki (2015)

$\alpha = 1.0$



Two thimbles

$\alpha = 3.0$



Single thimble

(red line) : thimble $\mathcal{J}_\sigma$

(blue line) : unstable-thimble $\mathcal{K}_\sigma$

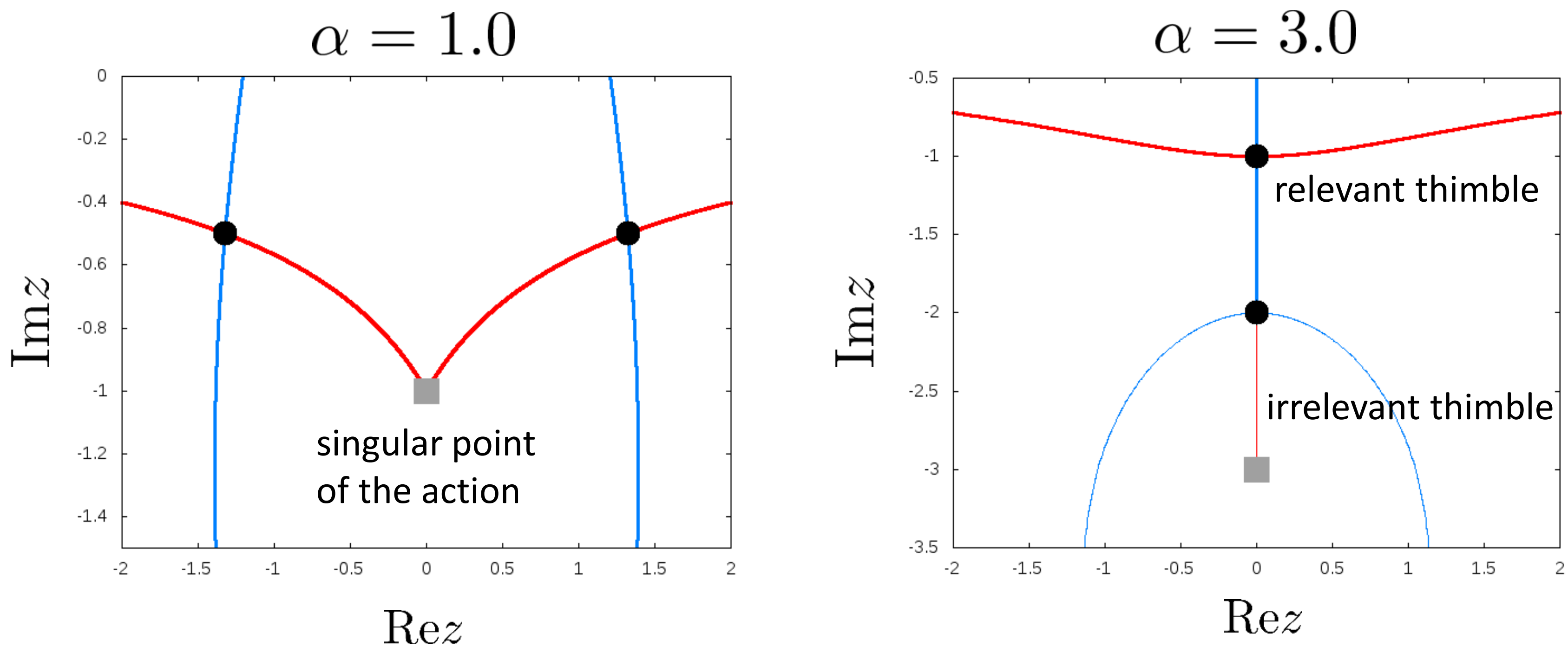
(black dot) : saddle point

(grey square) : singular point

A toy model

Cf) J. Nishimura, S. Shimasaki (2015)

$$Z = \int dx\ (x + i\alpha)^2 \mathrm{e}^{-x^2/2} \quad (\alpha \in \mathbb{R})$$



Singular point = End point of thimble

We focus on multi-thimble structure caused by singular points (zeros of “fermion determinant”).

Notations

$$Z_f = \int dx f(x) e^{-S(x)}$$

Partition function of "fermion+boson" theory

$$\langle O(x) \rangle_f = \frac{1}{Z_f} \int dx O(x) f(x) e^{-S(x)}$$

Expectation value

Namely, we denote

$$Z \equiv Z_1 = \int dx e^{-S(x)} \qquad \langle O(x) \rangle \equiv \langle O(x) \rangle_1$$

for "fermion-free" theory

Remark:

$$\langle f \rangle \langle O \rangle_f = \langle f O \rangle$$

Modification

Generalization of S. T., Takahiro M. Doi (2016)

Different "fermion+boson" theories are connected by

$$\langle f \rangle \langle O(x) \rangle_f + \langle g \rangle \langle O(x) \rangle_g = \langle f + g \rangle \langle O(x) \rangle_{f+g}$$

$\langle O \rangle_f$ An expectation value we want to know

g should be chosen so that

Z_g Z_{f+g} become single-thimble theories

How to find g(x)

$$\langle f\rangle\langle O(x)\rangle_f + \langle g\rangle\langle O(x)\rangle_g = \langle f+g\rangle\langle O(x)\rangle_{f+g}$$

$f = f(x;\alpha)$: "Fermionic determinant" of the original model

1. Find a parameter region (say $\alpha_1 \leq \alpha \leq \alpha_2$)
   in which the original model has a single-thimble structure

2. Choose $g(x;\beta) = f(x;\beta) \quad \alpha_1 \leq \beta \leq \alpha_2$
   (By definition, Z_g is single-thimble)

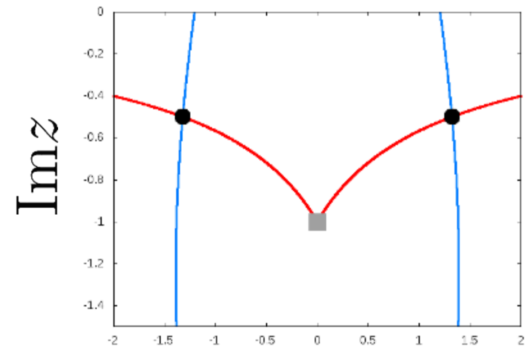
3. Find a parameter region (say $\beta_1 \leq \beta \leq \beta_2$)
   in which the modified model Z_{f+g} is single-thimble

At least, if $f = f(x;\alpha)$ and the action is a polynomial function of x, we find that the single-thimble model can be constructed in a following mechanism.

Application to the toy model

$$Z_f = \int dx f(x) e^{-x^2/2}$$

$$f(x) = (x + i\alpha)^2$$

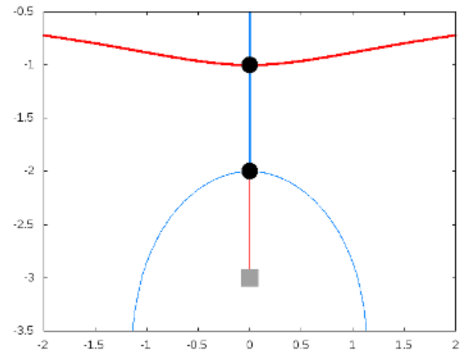


$\alpha = 1.0$

Multi-thimble

$$Z_g = \int dx g(x) e^{-x^2/2}$$

$$g(x) = (x + i\beta)^2$$



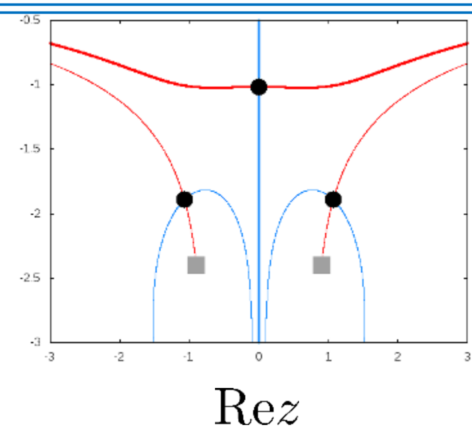
$\beta = 3.0$

Single-thimble

$$Z_{f+g} = \int dx (f(x) + g(x)) e^{-x^2/2}$$

Addition of $f(x)$ to $g(x)$ $\simeq$

Removing degeneracy of the singular point



$\alpha = 1.5$

$\beta = 3.3$

Single-thimble

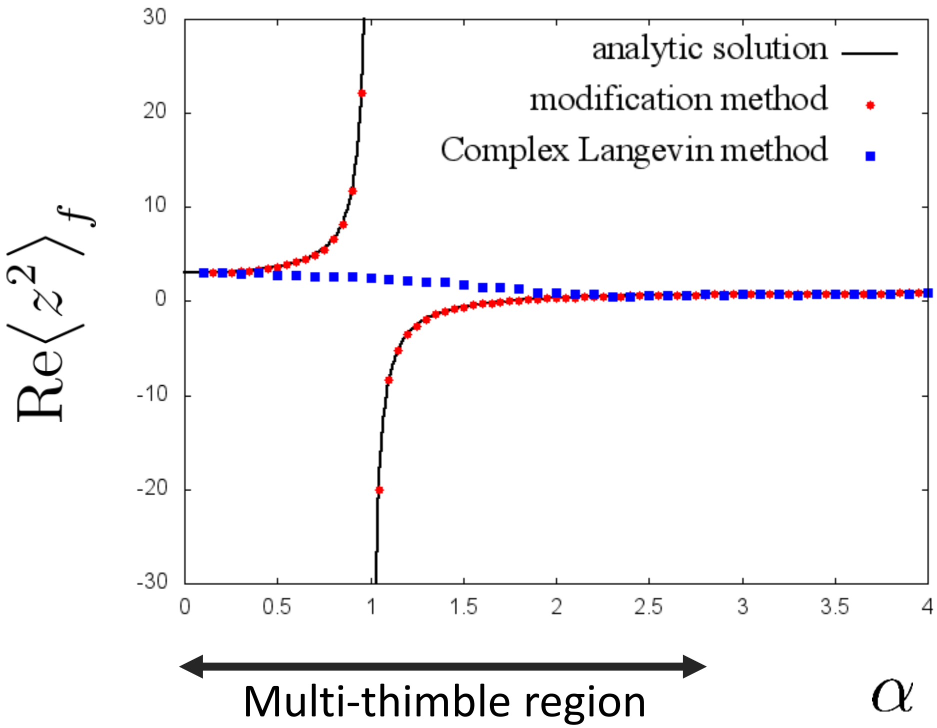
Computation of an expectation value

$$\langle f\rangle\left\langle z^2\right\rangle_f+\langle g\rangle\left\langle z^2\right\rangle_g=\langle f+g\rangle\left\langle z^2\right\rangle_{f+g}$$

$\left\langle z^2\right\rangle_f$ The expectation value we want to know.
It is difficult to obtain by naïve techniques due to the sign problem.

$\left\langle z^2\right\rangle_g, \left\langle z^2\right\rangle_{f+g}$

Quantities measured in **single-thimble** theory



$\langle f\rangle, \langle g\rangle, \langle f+g\rangle$

Quantities measured in fermion-free theory (Computed by usual Monte Carlo integration)

Discussion

Does our framework always work? … Unfortunately, no.

In principle, usual Monte Carlo simulation is applicable to compute $\langle f \rangle$

but it is difficult to do if $f(x)$ Is highly oscillating function

(e.g.) $f(x)$ Is a fermionic kernel for QCD

What should we do to avoid computing <f>?

$$\langle f \rangle \langle O(x) \rangle_f + \langle g_1 \rangle \langle O(x) \rangle_{g_1} = \langle f + g_1 \rangle \langle O(x) \rangle_{f+g_1}$$

$$\langle f \rangle \langle O(x) \rangle_f + \langle g_2 \rangle \langle O(x) \rangle_{g_2} = \langle f + g_2 \rangle \langle O(x) \rangle_{f+g_2}$$

Try two different modifications, and solve for $\langle O(x) \rangle_f$

One should carefully choose g_1, g_2 in order to minimize errors

Discussion

What should we do to avoid computing <f>?

$$\langle f \rangle \langle O(x) \rangle_f + \langle g \rangle \langle O(x) \rangle_g = \langle f + g \rangle \langle O(x) \rangle_{f+g}$$

$\langle g \rangle = 0$ ↓

$$\langle f \rangle \langle O(x) \rangle_f + \langle g O(x) \rangle = \langle f \rangle \langle O(x) \rangle_{f+g}$$

$\langle g O \rangle = 0$ ↓

$$\langle O(x) \rangle_f = \langle O(x) \rangle_{f+g}$$

Example: U(1) model

$$Z_f = \int_{-\pi}^{\pi} dx \cos x e^{\beta \cos x}$$

$$g(x) = i \sin x$$

$$O(x) = \cos(nx)$$

In this case, the expectation value of multi-thimble theory is directly obtained from the single-thimble theory without any additional measurements.

Summary

- We propose a new framework to obtain expectation values in a multi-thimble theory from a single-thimble theory.

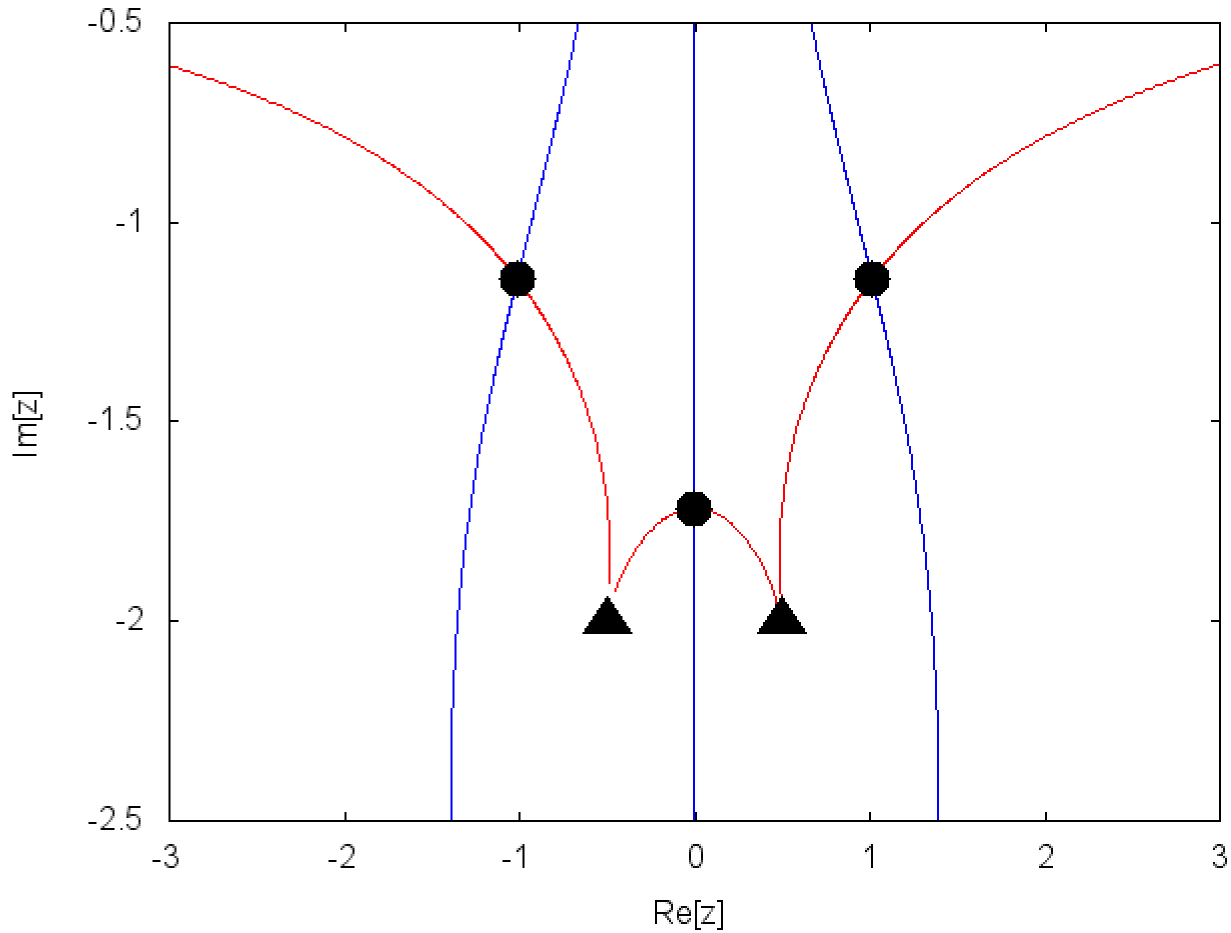
- We apply our framework to a toy-model, the Gaussian model. We show that two-thimble structure is modified to single-thimble structure.

Outlook

- It seems that the additive modification $Z_f \to Z_{f+g}$ where $g(x)$ has same form as $f(x)$ is quite useful to obtain a single-thimble theory. Why?
- It is important to study a special class of modification such that $\langle g \rangle \, , \langle gO \rangle = 0$
- We will also explore modifications of Thirring model and chiral random matrix theory.

Thank you for your attention!

Appendix



$$\alpha = 1.5$$

$$\beta = 2.5$$

$$Z_{f+g} = \int dx (f(x) + g(x)) e^{-x^2/2}$$

$$f(x) = (x + i\alpha)^2$$

$$g(x) = (x + i\beta)^2$$

Remaining sign problems

$$Z = \sum_{\sigma=1}^{N_{\rm sp}} n_\sigma \mathrm{e}^{-i{\rm Im}S(z_\sigma)} \int dx \mathrm{e}^{i \arg \det J(x)} \mathrm{e}^{-S_{\rm eff}(x)}$$

Global phase factor Residual phase factor

$$S_{\rm eff}(x) = {\rm Re}S(z(x)) - \ln|\det J(x)|$$

$J(x) = \frac{\partial z}{\partial x}$: Jacobian

Sign problem can occur due to interference of the global phase factors

Sign problem

From a practical point of view…

$$S(x) = \mathrm{Re}S(x) + i\mathrm{Im}S(x)$$

$$\frac{1}{Z}\int dx O(x)\mathrm{e}^{-S(x)} = \frac{1}{Z}\int dx \left(O(x)\mathrm{e}^{-i\mathrm{Im}S(x)}\right)\mathrm{e}^{-\mathrm{Re}S(x)}$$

$$\sim \frac{1}{N}\sum_{i=1}^{N} O(x_i)\mathrm{e}^{-i\mathrm{Im}S(x_i)}$$

x_i is a random variable with the distribution $P(x) \propto \mathrm{e}^{-\mathrm{Re}S(x)}$

Sign problem = we cannot compute this quantity accurately!
(typically, MC gives 0 due to the phase oscillation)