An improved complex Langevin method motivated by Lefschetz thimbles

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in collaboration with
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"An improvement in complex Langevin dynamics
from a view point of Lefschetz thimbles", **arXiv:1508.04231[hep-lat]**

CPHEHIC, Oct. 5, 2015, YITP, Kyoto

Motivation

Goal

First principle calculation of a theory with a complex action:

$$Z = \int dx e^{-S(x)} \qquad \text{with} \quad S(x) \in \mathbb{C}$$

Sign problem

Boltzmann factor $e^{-S(x)}$ is no longer
a probability distribution when the action is complex.

Physical application

- QCD at finite chemical potential
- QCD in external electric field
- All real time problems (far from equilibrium)
- Frustrated spin systems
- Hubbard model away from half-filling

and so on...

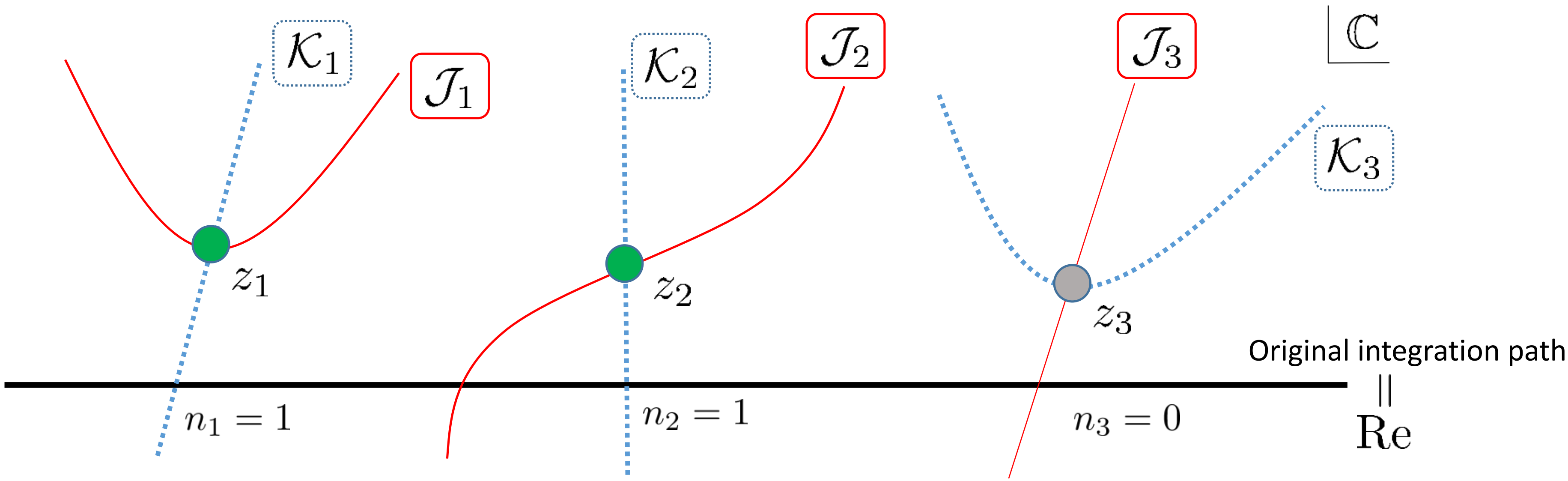
Lefschetz thimble: a candidate to solve the sign problem

F. Pham, Proc. Symp. Pure Math. 40, 319 (1983).
E. Witten, arXiv:1001.2933 [hep-th]

Method of Lefschetz thimbles = A generalization of the method of steepest descent

$$\underbrace{Z = \int dx\, \mathrm{e}^{-S(x)}}_{\text{Original partition fnc.}} = \underbrace{\sum_{\sigma=1}^{N_{\mathrm{th}}} n_\sigma \mathrm{e}^{-i\mathrm{Im}S(z_\sigma)} \int_{\mathcal{J}_\sigma} dz\, \mathrm{e}^{-\mathrm{Re}S(z)}}_{\text{Decomposition to Lefschetz thimbles}} \qquad x \in \mathbb{R}, \quad S(x) \in \mathbb{C}$$

Example of two-thimble case with $N_{\mathrm{th}} = 3$



Global sign problem in multi-thimble system

In multi-thimble case, there is cancelation between thimbles

Example: 2-thimble case

$$Z = \mathrm{e}^{-i\mathrm{Im}S(z_1)} \int_{\mathcal{J}_1} dz\ \mathrm{e}^{-\mathrm{Re}S(z)} + \mathrm{e}^{-i\mathrm{Im}S(z_2)} \int_{\mathcal{J}_2} dz\ \mathrm{e}^{-\mathrm{Re}S(z)}$$

Sign problem remains as a cancelation between thimbles (Global sign problem)

Note: There is no global sign problem in single-thimble structure.

Special case: 1-thimble case

$$Z = \mathrm{e}^{-i\mathrm{Im}S(z_1)} \int_{\mathcal{J}_1} dz\ \mathrm{e}^{-\mathrm{Re}S(z)}$$

Only single thimble contributes to the partition function

→ No cancelation between thimbles (No global sign problem)

Complex Langevin dynamics

complex Langevin dynamics(CL): stochastic quantization for complex actions

Complex Langevin equation

$$\frac{dz}{dt} = -\frac{\partial S(z)}{\partial z} + \eta$$

$$\langle \eta(t) \rangle = 0$$

$$\langle \eta(t)\eta(t') \rangle = 2\delta(t - t')$$

⇒ noise average **?** expectation value

$$\langle \mathcal{O}(x(t)) \rangle \xrightarrow{t\to\infty} \int dx \mathcal{O}(x) e^{-S}/Z$$

Parisi, Wu (1981)

Parisi (1983)
Klauder, Petersen (1985)
Ambjorn, S.K. Yang (1985)

Properties of CL

- Not heavy numerical cost to perform CL.
- Sometimes, CL gives incorrect results. ← G. Aarts, E. Seiler, and I.-O. Stamatescu (2010); G. Aarts, F. A. James, E. Seiler, I.-O. Stamatescu (2011); J. Nishimura and S. Shimasaki (2015)
- Related to the method of Lefschetz thimble

Importance sampling on a single thimble

⇓

Complex Langevin dynamics gives the correct results.

Our strategy: modification method

TMD and S. Tsutsui, arXiv:1508.04231 [hep-th]

1. Consider a theory with following form.

original theory: $Z = \int_{D_0} dx\ f(x) e^{-S_q(x)}$ with $f(x) \in \mathbb{C}, \quad S_q(x) \in \mathbb{R}$

2. Modify the theory so that it is calculable.

modified theory: $\tilde{Z} = \int_{D_0} dx\ (f(x) + ig(x)) e^{-S_q(x)}$ with $g(x) \in \mathbb{R}$

3. Reconstruct the observable in the original theory from observables in different theories.

Modification formula: connecting observables in different theory

$$\langle \mathcal{O} \rangle_Z = \mathrm{Re} \langle \mathcal{O} \rangle_{\tilde{Z}} - \frac{\langle g \rangle_{Z_q}}{\langle f \rangle_{Z_q}} \mathrm{Im} \langle \mathcal{O} \rangle_{\tilde{Z}}$$

valid for $g(x),\ \mathcal{O}(x) \in \mathbb{R},\ x \in \mathbb{R}$

Modified theory:

$\langle \mathcal{O} \rangle_{\tilde{Z}}$ is obtained by complex Langevin

Quenched theory: Monte Carlo method is applicable.

$$Z_q = \int_{D_0} dx\ e^{-S_q(x)}$$

Application of the modification method to a toy model

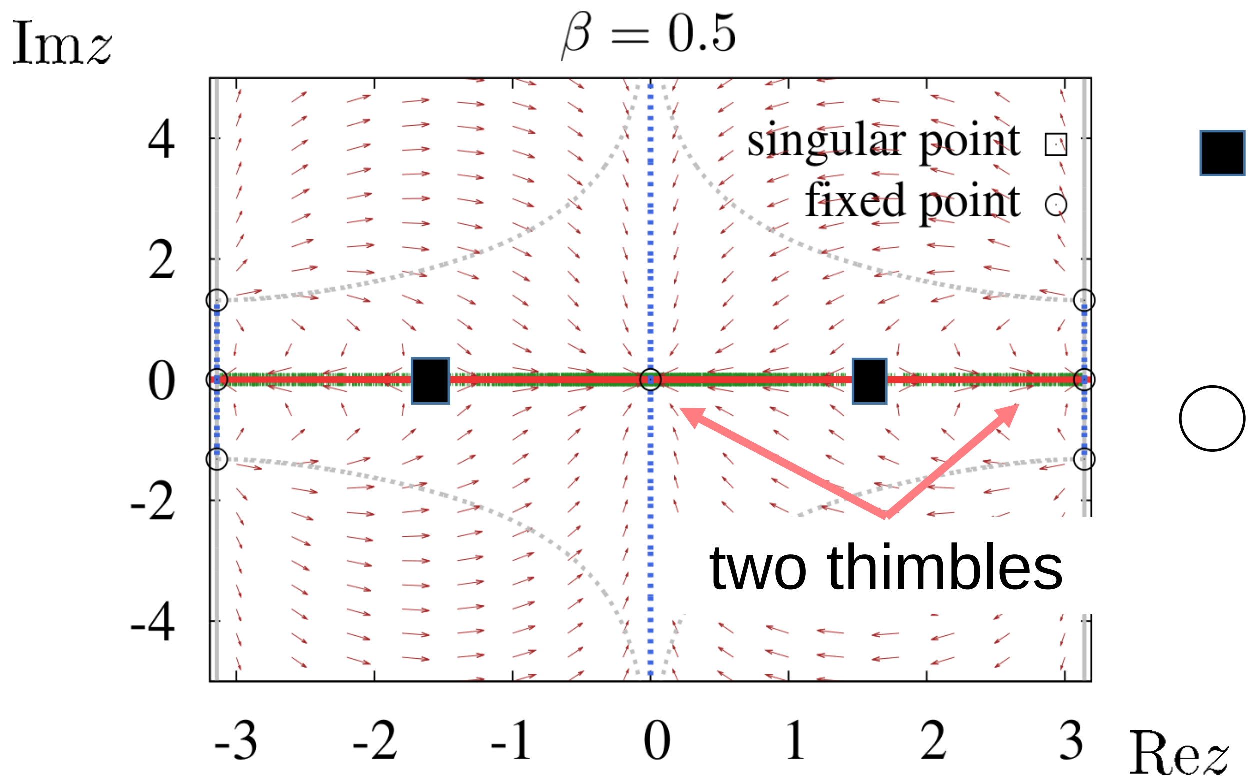
arXiv:1508.04231

A toy model: cosine model

J. Ambjorn, M. Flensburg, and C. Peterson, Nucl.Phys. B275, 375 (1986).

$$Z = \int_{-\pi}^{\pi} dx \cos x \; e^{\beta \cos x}$$: From U(1) gauge theory on 2-dim. lattice

$$= \int_{-\pi}^{\pi} dx e^{-S(x)}, \qquad S(x) = -\beta \cos x + \log(\cos x)$$



■ : singular points determined by

$$\cos z = 0$$

○ : saddle points determined by

$$\frac{\partial S}{\partial z} = \beta \sin z - \tan z = 0$$

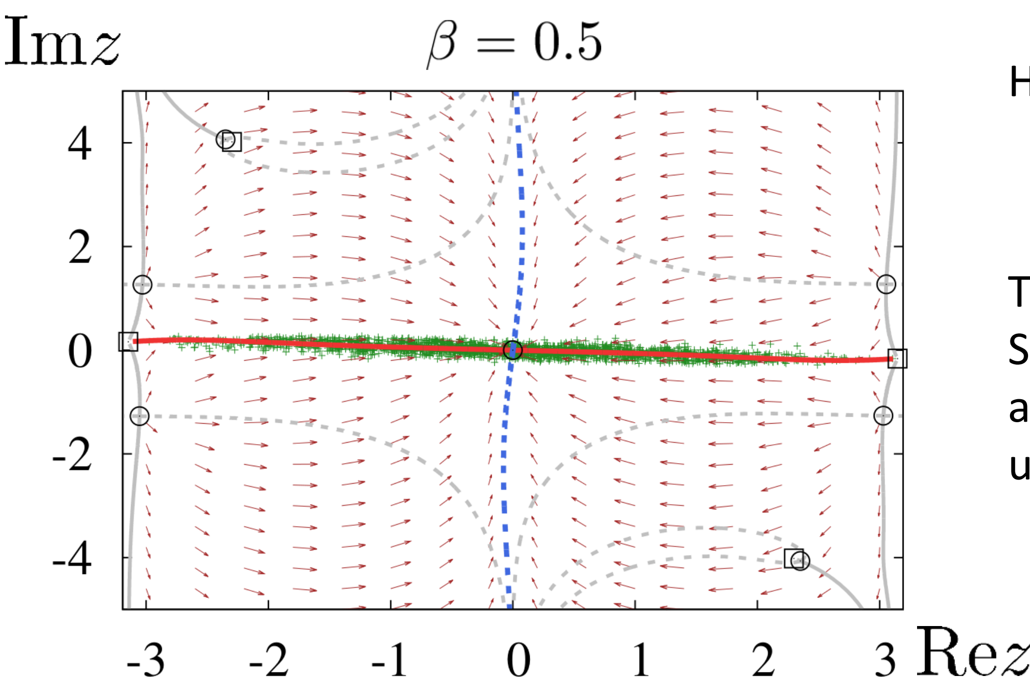
How to modify? How to choose g(x)?

modified theory: $\tilde{Z} = \int_{-\pi}^{\pi} dx\ (\cos x + \underline{ig(x)}) \mathrm{e}^{\beta \cos x}$ with $g(x) \in \mathbb{R}$

Criterions to obtain the observable $\langle \mathcal{O} \rangle_{\tilde{Z}}$ correctly.

1: Single-thimble structure:
The modified theory $\tilde{Z}$ has a single thimble to avoid the global sign problem.

2: Importance sampling on the (single) thimble
The configuration {z} in the complex Langevin dynamics are distributed around the thimble.



Here, we choose

$$g(x) = (x - \pi)(x + \pi)$$

The above criterions are satisfied.
So, we can obtain the modified observable and reconstruct the original observable using the modification formula.

$$\langle \mathcal{O} \rangle_Z = \mathrm{Re} \langle \mathcal{O} \rangle_{\tilde{Z}} - \frac{\langle g \rangle_{Z_q}}{\langle f \rangle_{Z_q}} \mathrm{Im} \langle \mathcal{O} \rangle_{\tilde{Z}}$$

Final results of modification method in cosine model

Modification formula:

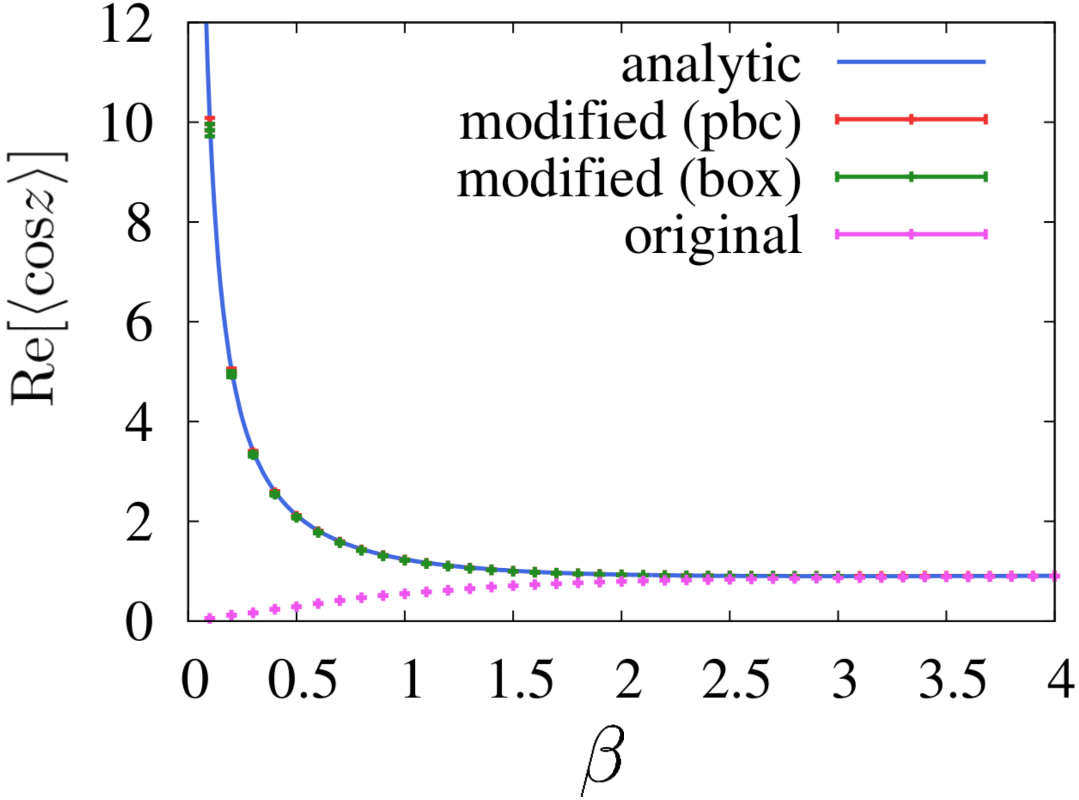
$$\langle \mathcal{O} \rangle_Z = \mathrm{Re}\langle \mathcal{O} \rangle_{\tilde{Z}} - \frac{\langle g \rangle_{Z_\mathrm{q}}}{\langle f \rangle_{Z_\mathrm{q}}} \mathrm{Im}\langle \mathcal{O} \rangle_{\tilde{Z}}$$

$$Z = \int_{-\pi}^{\pi} dx \cos x \, \mathrm{e}^{\beta \cos x} \qquad f(x) = \cos x$$

$$\tilde{Z} = \int_{-\pi}^{\pi} dx \, (\cos x + i\tau g(x)) \mathrm{e}^{\beta \cos x}$$

with $g(x) = (x - \pi)(x + \pi)$

$$\mathcal{O}(x) = \cos x$$



- Our modification method reproduces the correct result while the original complex Langevin dynamics fails to give it.
- There is no dependence of boundary conditions.

Summary

1

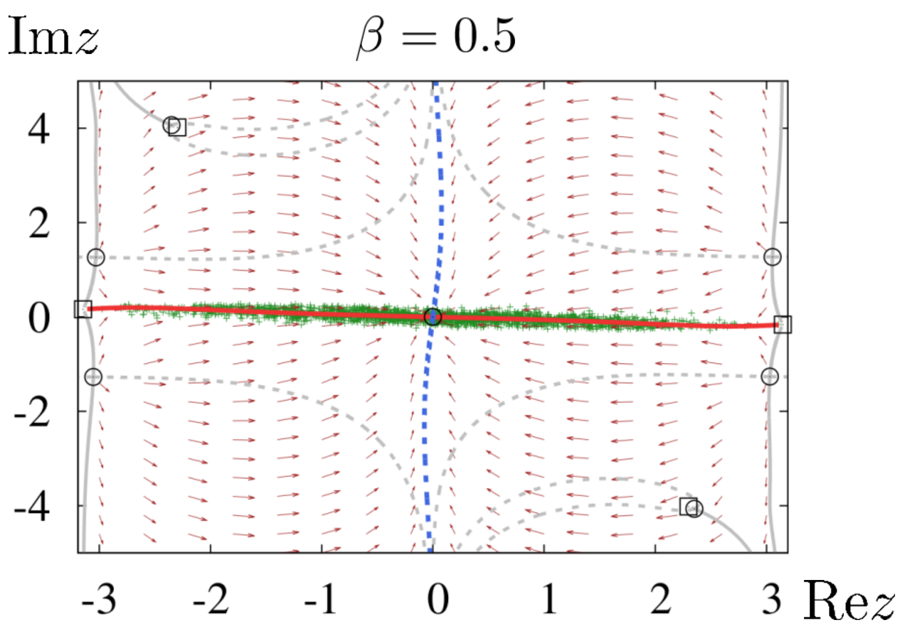
We develop a new method, modification method
motivated by the method of Lefschetz thimble.

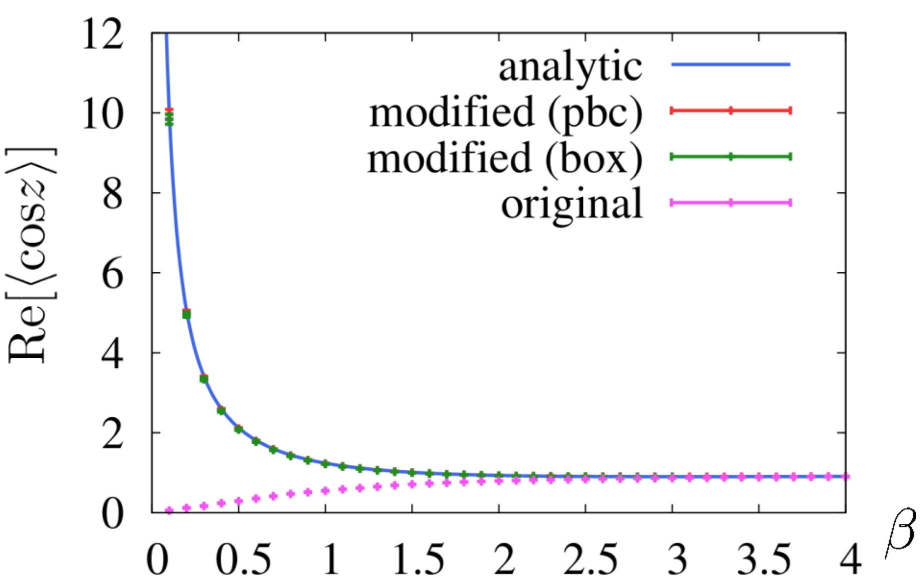
2

We apply our method to the cosine model, where the naive complex Langevin dynamics fails to give the correct results.

3

We certainly could modify the original theory
so that the modified theory has an only thimble,
and then the modification method reproduces the correct results.



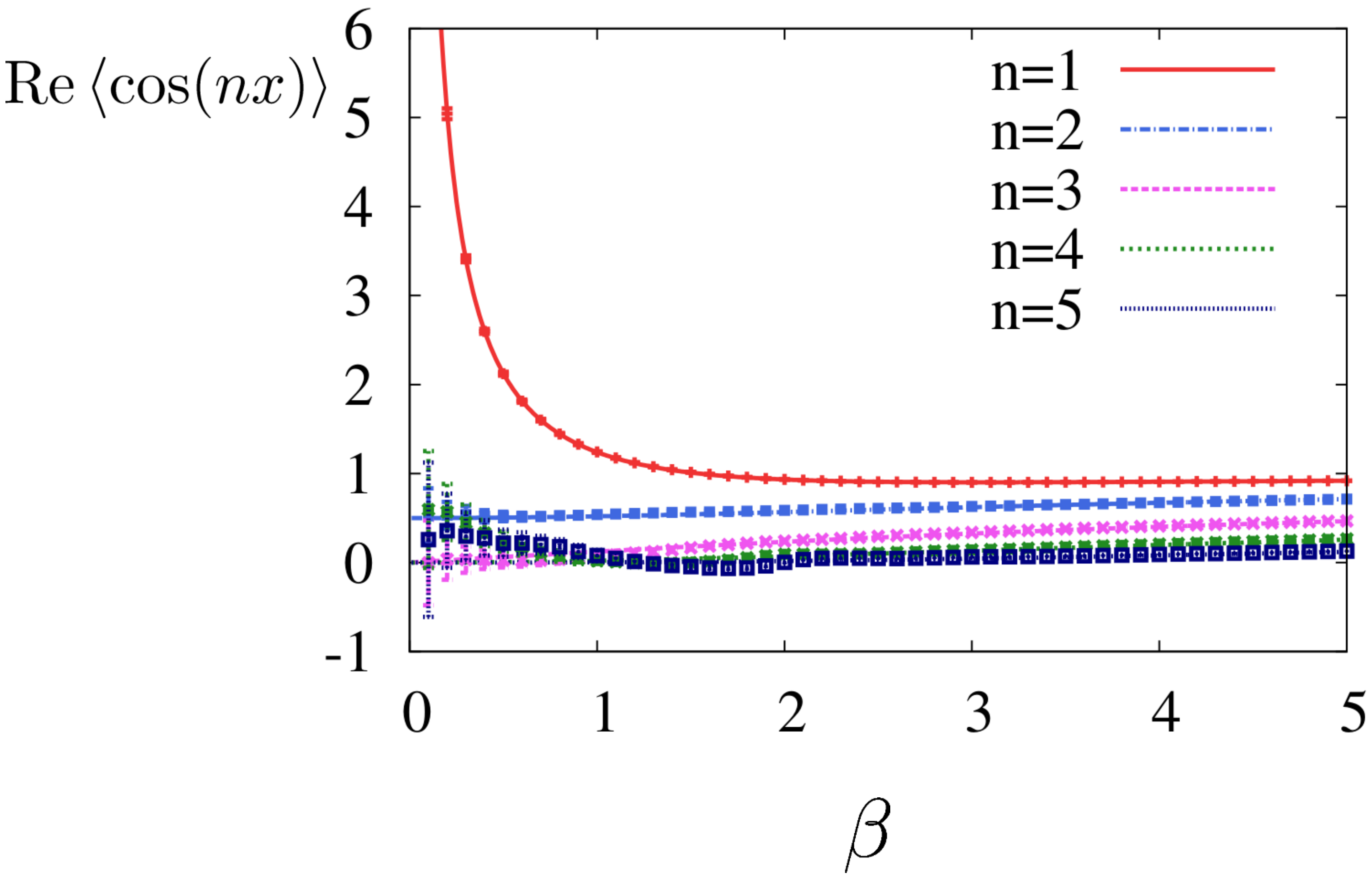


Outlook

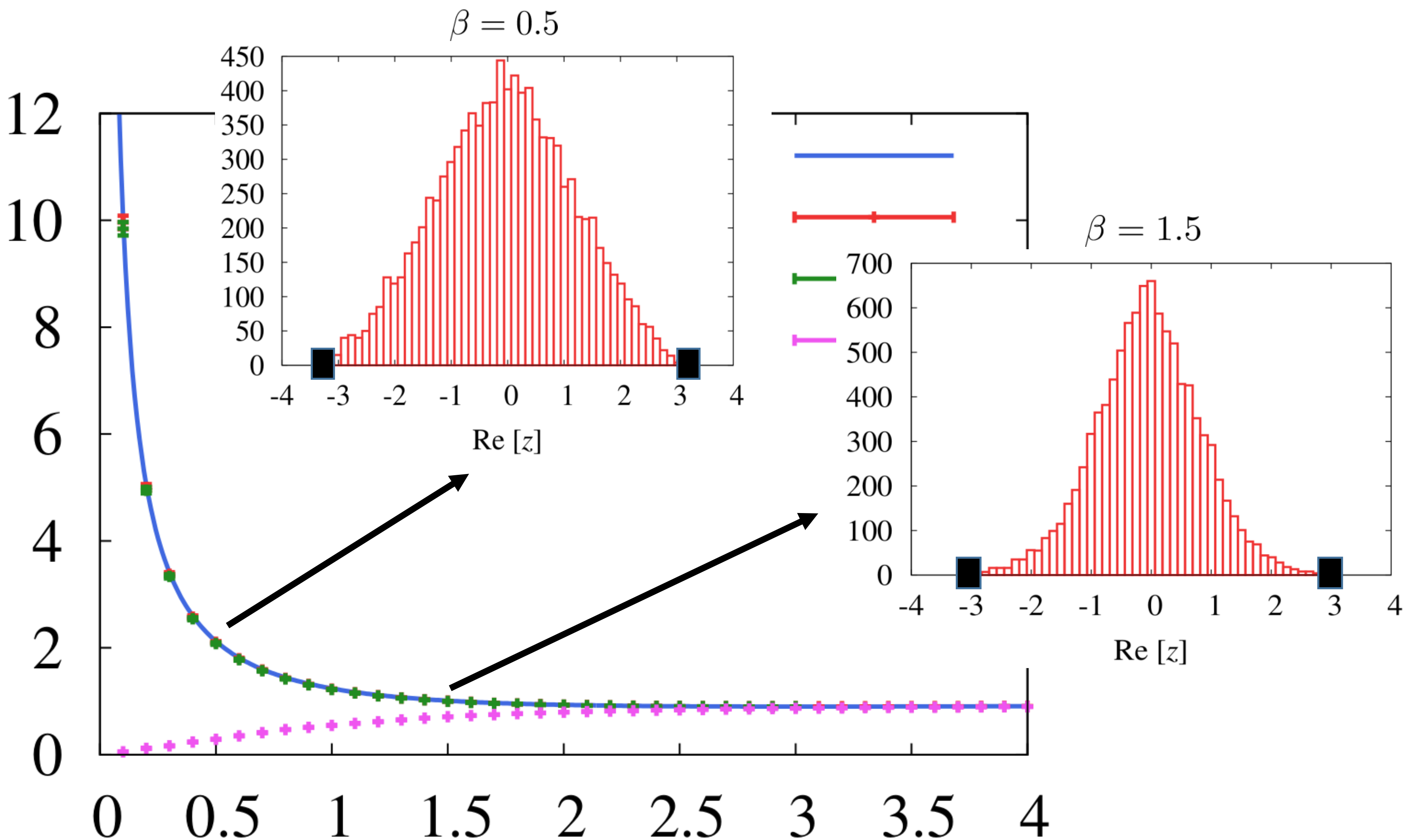
- More systematic ways to find an appropriate modification g(x) is desired.
- It is also interesting to apply our method to a model which shows phase transitions.
- Other model which has multi-dimension more than 1.

Appendix

higher cumulants



singularity



Remained problem in modification method

Modification formula:

$$\langle \mathcal{O} \rangle_Z = \mathrm{Re}\langle \mathcal{O} \rangle_{\tilde{Z}} - \frac{\langle g \rangle_{Z_\mathrm{q}}}{\langle f \rangle_{Z_\mathrm{q}}} \mathrm{Im}\langle \mathcal{O} \rangle_{\tilde{Z}}$$

$\langle f \rangle_{Z_\mathrm{q}}$ is nothing but the original partition function :

$$\langle f \rangle_{Z_\mathrm{q}} = \frac{\int_{D_0} dx\ f(x) \mathrm{e}^{-S_\mathrm{q}(x)}}{\int_{D_0} dx\ \mathrm{e}^{-S_\mathrm{q}(x)}} = \frac{Z}{Z_\mathrm{q}}$$

In principle, Monte Carlo method is applicable to calculate $\langle f \rangle_{Z_\mathrm{q}}$ because of real $S_\mathrm{q}(x) \in \mathbb{R}$, but it is difficult to calculate it with sufficient accuracy if $f(x)$ is highly oscillating function.

(Example: QCD with large chemical potential・・・ $f(x)$ is fermionic kernel K[U])

$$\langle g \rangle_{Z_\mathrm{q}} = \frac{\int_{D_0} dx\ g(x) \mathrm{e}^{-S_\mathrm{q}(x)}}{\int_{D_0} dx\ \mathrm{e}^{-S_\mathrm{q}(x)}}$$

If $\langle g \rangle_{Z_\mathrm{q}} = 0$, we don't have to calculate $\langle f \rangle_{Z_\mathrm{q}}$.
$\langle g \rangle_{Z_\mathrm{q}} = 0$ can be satisfied using symmetries in the quenched theory.

theories	quenched action	symmetries of S_q
cosine model	$S_\mathrm{q}(x) = \beta \cos x$	parity (x→-x)
QCD	pure YM action	・gauge symmetry(Elitzur's theorem) ・Z_3 (Center) symmetry ・C, P and T symmetry ・Space-time symmetry

An example: complex Langevin dynamics on cosine model

J. Ambjorn, M. Flensburg, and C. Peterson, Nucl.Phys. B275, 375 (1986).

Add 0 to the partition function;

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

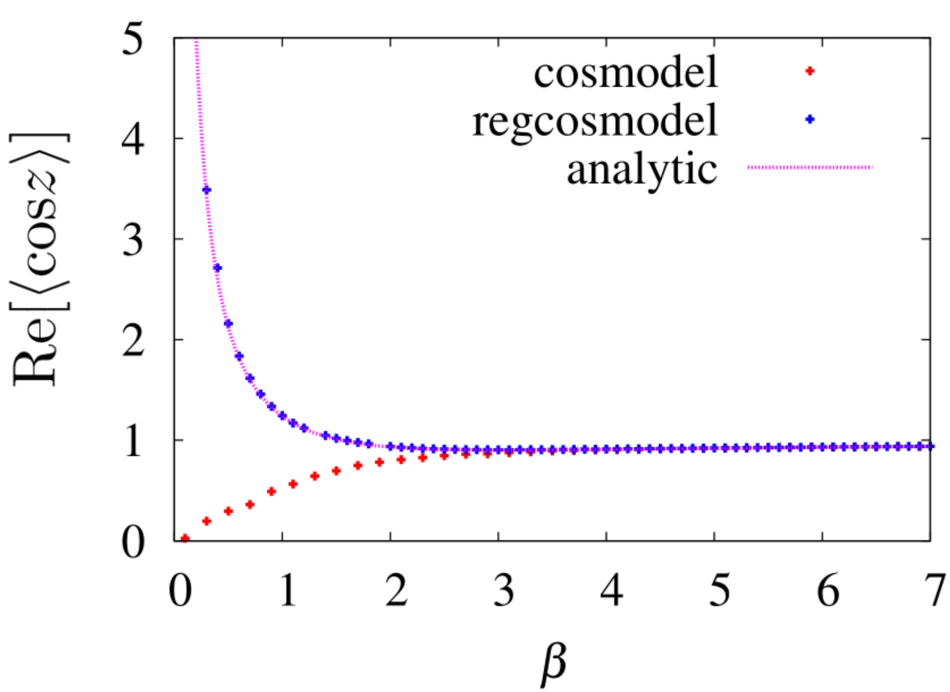
$$0 = \int_{-\pi}^{\pi} dx \; i \sin x \mathrm{e}^{\beta \cos x}$$

Add →

$$Z = \int_{-\pi}^{\pi} dx \mathrm{e}^{ix} \mathrm{e}^{\beta \cos x}$$:"regularized cosine model"

$$= \int_{-\pi}^{\pi} dx \mathrm{e}^{-S_{\mathrm{reg}}(x)}, \qquad S_{\mathrm{reg}}(x) = -\beta \cos x - ix$$

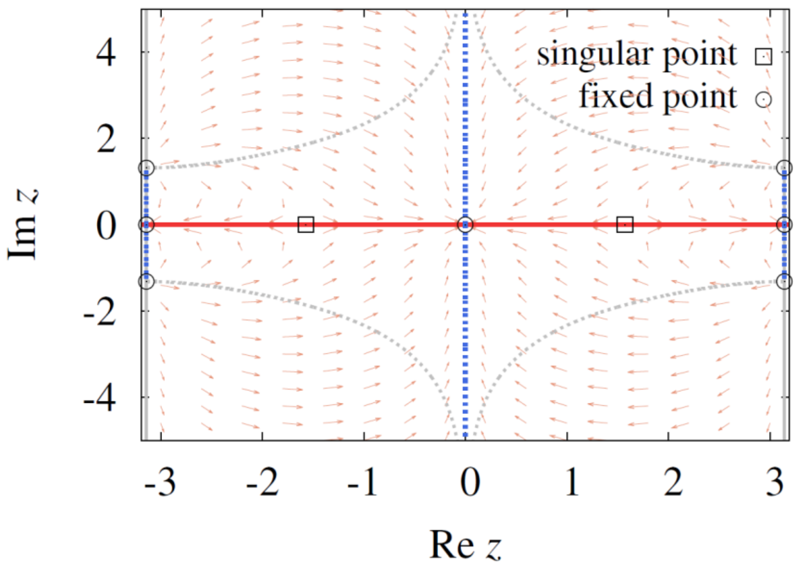
In fact, the complex Langevin dynamics of regularized cosine model gives correct result.



Thimble structure in cosine and regularized cosine models

our calculation

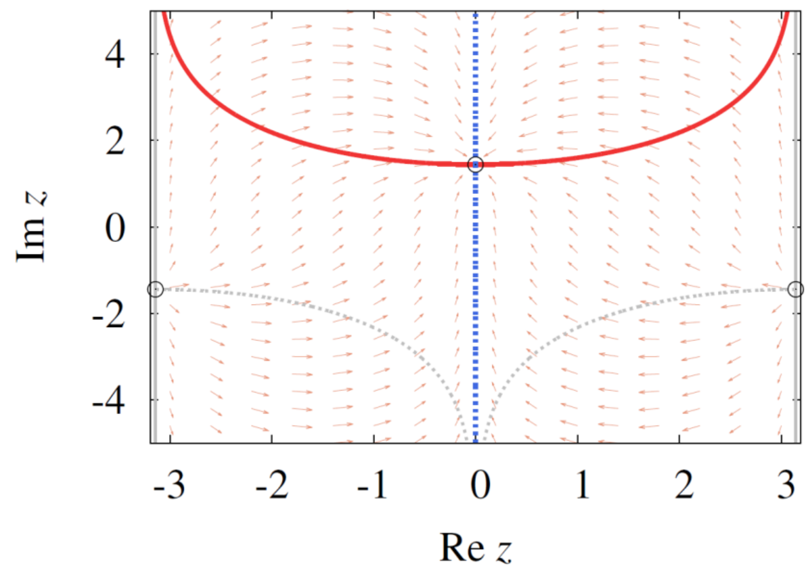
cosine model with $\beta = 0.5$



2 thimble structure:
complex Langevin dynamics doesn't work well due to the global sign problem.

Singular point is endpoint of thimble.

regularized model with $\beta = 0.5$



1 thimble structure:
complex Langevin dynamics works well.

○ : fixed point

□ : singular point

→ : complex Langevin flow

— : stable thimble $\mathcal{J}_\sigma$

···· : unstable thimble $\mathcal{K}_\sigma$

Complex Langevin dynamics

$$\langle \mathcal{O}(z(t)) \rangle \overset{?}{\to} \frac{1}{Z} \int dx\ \mathcal{O}(x) \mathrm{e}^{-S(x)} \qquad (t \to \infty)$$

Q. Is stochastic quantization correct even with complex action?

A. It depends. Sometimes, complex Langevin dynamics gives the incorrect result.

- Some criteria for correctness of the complex Langevin dynamics are proposed from the view point of Fokker-Planck equation.

  G. Aarts, E. Seiler, and I.-O. Stamatescu, Phys.Rev. D81, 054508 (2010).
  G. Aarts, F. A. James, E. Seiler, and I.-O. Stamatescu, Eur.Phys.J. C71, 1756 (2011).
  J. Nishimura and S. Shimasaki, Phys. Rev. D92, 011501 (2015).

- Some practical methods are invented to improve complex Langevin method.
  - Adaptive step-size method

    G. Aarts, F. A. James, E. Seiler, and I.-O. Stamatescu, Phys.Lett. B687, 154 (2010).
    J. Flower, S. W. Otto, and S. Callahan, Phys.Rev. D34, 598 (1986).
  - Gauge cooling method

    E. Seiler, D. Sexty, and I.-O. Stamatescu, Phys.Lett. B723, 213 (2013).
  - Changing integration-variables

    A. Mollgaard and K. Splittor, Phys.Rev. D91, 036007 (2015).

However, it is still difficult to expect when complex Langevin dynamics gives correct results.

Sign problems in the Lefschetz thimble formalism

- Residual sign problem

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

$$= \sum_\sigma n_\sigma \mathrm{e}^{-i\mathrm{Im}S(z_\sigma)} \int ds_\sigma J(s_\sigma) \mathrm{e}^{-\mathrm{Re}S(z(s_\sigma))}$$

s: parameter of the thimble $\mathcal{J}_\sigma$

J(s): Jacobian

Jacobian can be complex

⇒ Monte Carlo method is not simply applicable.....

- Global sign problem (2-thimble example)

$$Z = n_1 \mathrm{e}^{-i\mathrm{Im}S(z_1)} \int_{\mathcal{J}_1} dz\ \mathrm{e}^{-\mathrm{Re}S(z)} + n_2 \mathrm{e}^{-i\mathrm{Im}S(z_2)} \int_{\mathcal{J}_2} dz\ \mathrm{e}^{-\mathrm{Re}S(z)}$$

$\mathrm{Im}S(z_\sigma)$ of different thimbles is not always the same.

⇒ There is cancelation between different thimbles.

Note: there is no global sign problem in the case of the single thimble.

Thimble structure in the modification method

The modified theory: $$\tilde{Z} = \int_{D_0} dx\ (f(x) + i\tau g(x))\mathrm{e}^{-S_\mathrm{q}(x)}$$

In order to draw thimble, singular point and fixed point are required.

singular point z_s : $$f(z_\mathrm{s}) + i\tau g(z_\mathrm{s}) = 0$$

fixed point z_f : $$S'(z_\mathrm{f}) - \frac{f'(z_\mathrm{f}) + i\tau g'(z_\mathrm{f})}{f(z_\mathrm{f}) + i\tau g(z_\mathrm{f})} = 0$$

prime (‘) means the derivative with respect to z.

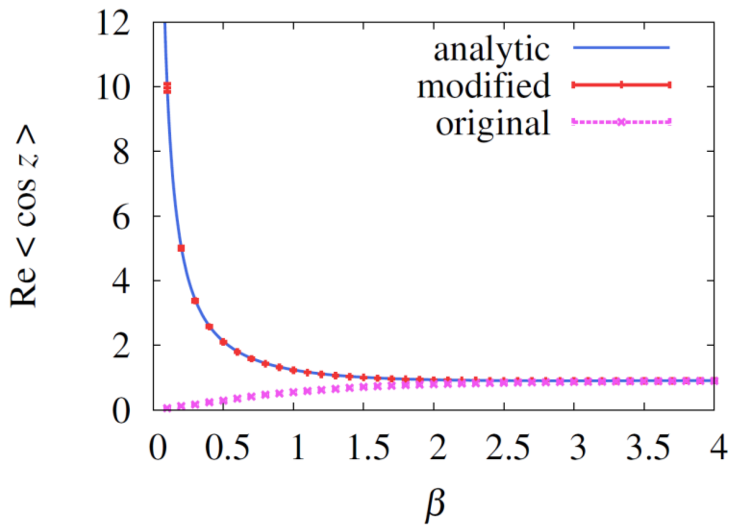
In a practical sense, it is useful to see the τ evolution of singular and fixed points.

singular point z_s : $$\frac{dz_\mathrm{s}}{d\tau} = \frac{-ig(z_\mathrm{s})}{f'(z_\mathrm{s}) + i\tau g'(z_\mathrm{s})}$$

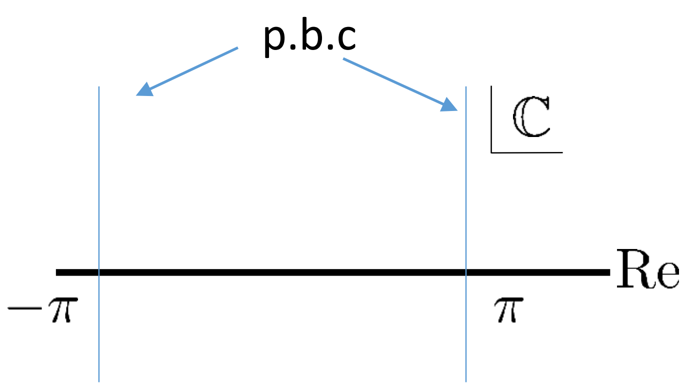
fixed point z_f : $$\frac{dz_\mathrm{f}}{d\tau} S''_\mathrm{q} = \frac{1}{(f + i\tau g)^2}\Big\{ ifg' - if'g + \frac{dz_f}{d\tau}(f'' + i\tau g'')(f + i\tau g) - (f' + i\tau g')^2 \Big\}$$

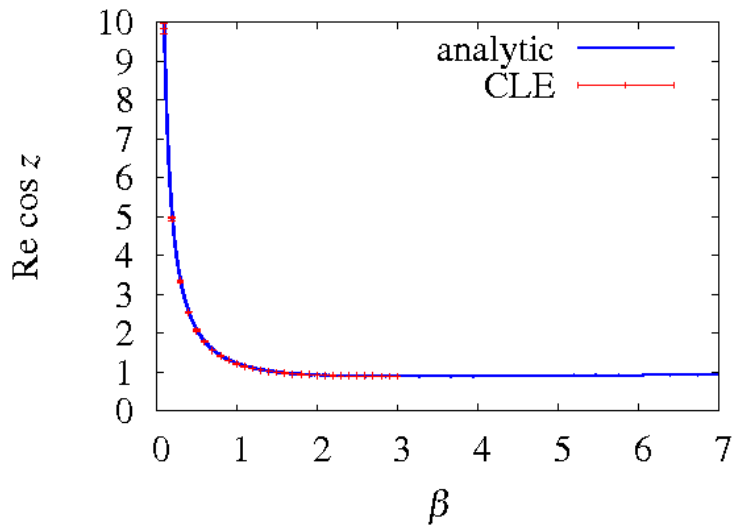
Dependence of boundary condition

- We have performed the complex Langevin dynamics in the modified cosine model with 2 types boundary condition.



periodic boundary condition at $\mathrm{Re}z = \pm\pi$.





Box boundary condition:
small repulsive force at $\mathrm{Re}z = \pm\pi$