Optimized flow for generalized Lefschetz thimble method

Katsuta Sakai (KEK → Tokyo Medical and Dental University)

In collaboration with

Jun Nishimura (KEK & SOKENDAI),

Atis Yosprakob (Niigata University)

In preparation

KEK Theory workshop 2022 (Online(KEK), Dec. 7, 2022)

1. Introduction

Monte-Carlo (MC) simulation…… An efficient method to have numerical integrations

Ex) path integral

$$\langle \mathcal{O} \rangle \equiv \frac{\int dx\, e^{-S(x)} \mathcal{O}(x)}{\int dx\, e^{-S(x)}} \quad \Rightarrow \quad \langle \mathcal{O} \rangle = \sum_{i=1}^{N_{\rm sample}} \mathcal{O}(x^{(i)})$$

With $\{x^{(i)}\}_i$ generated by $p(x^{(i)}) = \frac{e^{-S(x^{(i)})}}{\int dx e^{-S(x)}}$

weight → probability dist.

MC with complex weight (⇔ $S \in \mathbb{C}$)

→ Reweighting? $\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} e^{-i{\rm Im}\, S} \rangle}{\langle e^{-i{\rm Im}\, S} \rangle}, \quad p(x^{(i)}) = \frac{e^{-{\rm Re}\, S(x^{(i)})}}{\int dx e^{-{\rm Re}\, S(x)}}$

→ The phase $e^{-i{\rm Im}\, S}$ oscillates; convergence is exponentially slow

Sign problem : Obstacle to study on real-time dynamics, QCD with finite density and theta term, *etc*.

1. Introduction

To circumvent the sign problem…

Generalized thimble method (GTM) [Alexandru-Basar-Bedaque, '15]
[Alexandru-Basar-Bedaque-Ridgway-Warrington, '16]

Complexify variables & deform integral contour with the holomorphic gradient eq.

Cf.) Picard-Lefschetz theory

$$x \to z(x,\sigma) \quad \text{with} \quad \frac{\partial z}{\partial \sigma} = \overline{\frac{\partial S(z)}{\partial z}}, \quad z(x,0) = x$$

$$\Rightarrow \quad \frac{\partial S(z(x,\sigma))}{\partial \sigma} = \left| \frac{\partial S}{\partial z} \right|^2 > 0$$

Along the flow , $e^{-i\mathrm{Im}\, S}$: constant

$e^{-\mathrm{Re}\, S}$: decrease

1. Introduction

To circumvent the sign problem…

Generalized thimble method (GTM) [Alexandru-Basar-Bedaque, '15] [Alexandru-Basar-Bedaque-Ridgway-Warrington, '16]

Complexify variables & deform integral contour with the holomorphic gradient eq.

Cf.) Picard-Lefschetz theory

$$x \to z(x,\sigma) \quad \text{with} \quad \frac{\partial z}{\partial \sigma} = \overline{\frac{\partial S(z)}{\partial z}}, \quad z(x,0) = x$$

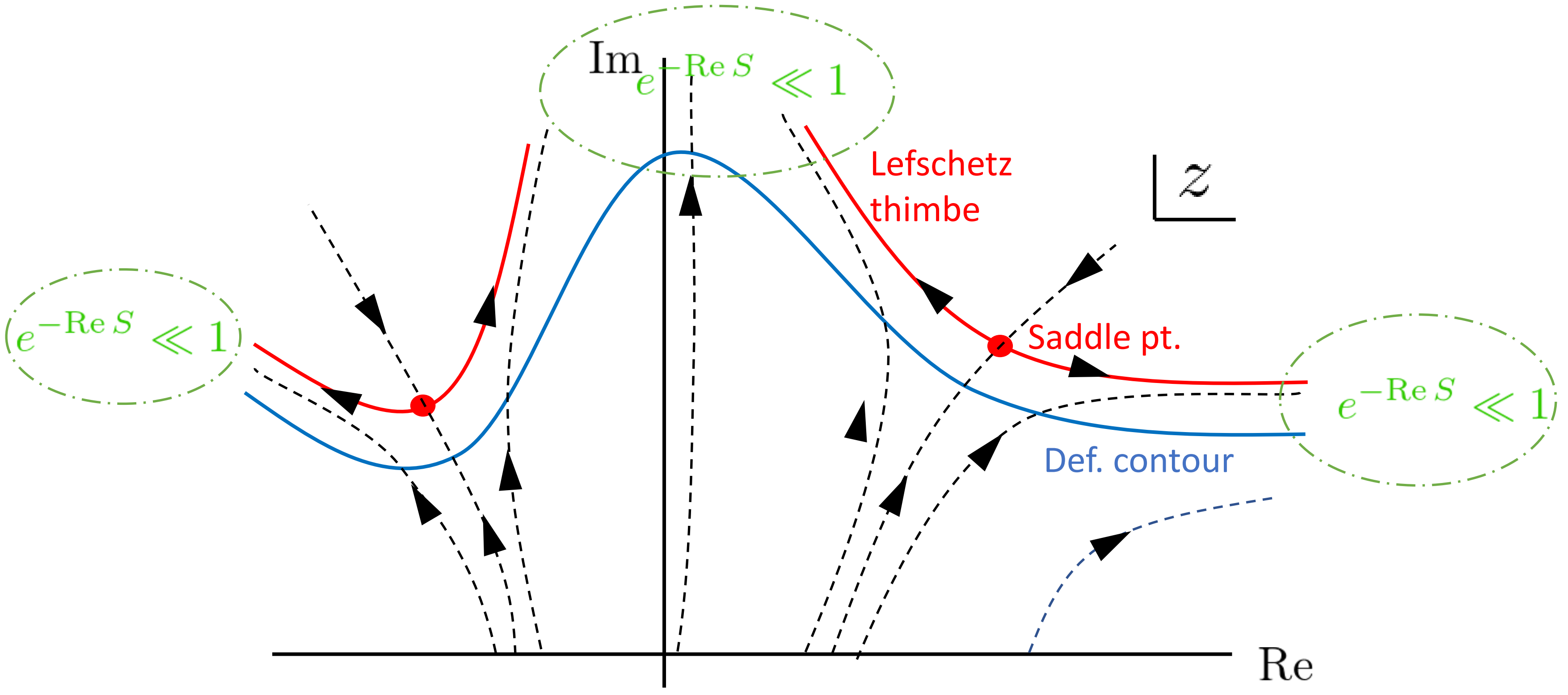
$$\Rightarrow \quad \frac{\partial S(z(x,\sigma))}{\partial \sigma} = \left|\frac{\partial S}{\partial z}\right|^2 > 0$$

Along the flow , $e^{-i\mathrm{Im}\,S}$: constant

$e^{-\mathrm{Re}\,S}$: decrease

The deformed contour approaches a set of steepest descent curves (Lefschetz thimbles)

→ spanned by expanded nearly-constant-phase regions



1. Introduction

Why expansive map?

- flow eq. for deviation $\delta z_j = z_j - z'_j$: $\dfrac{\partial(\delta z_j)}{\partial \sigma} = \overline{H_{jk}} \overline{\delta z_k}$

  Hessian

➡ Roughly, exponential expansion with rates "singular values of $\overline{H}$ "

Subtlety in GTM

- Expansion rates differ mode by mode (high-energy mode → large expansion rate)

  ➡ Suitable region of flow time (to solving the sign prob. & Ergodicity prob.) also differ

- In the standard GTM, we move the sampling pt. on the original or deformed contour with mode-independent step size

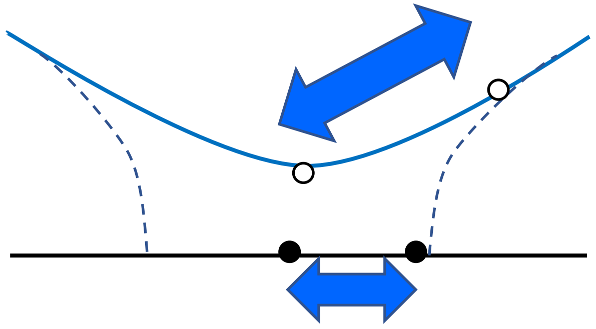
1. Introduction

Then, when we take the sampling with multimode…

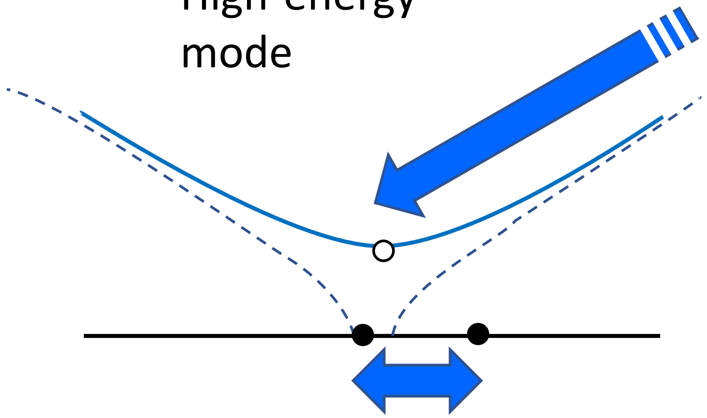
Case a) Sampling point on the original contour

[Alexandru-Basar-Bedaque, ’15]
[Alexandru-Basar-Bedaque-Ridgway-Warrington, ’16]

Low-energy mode

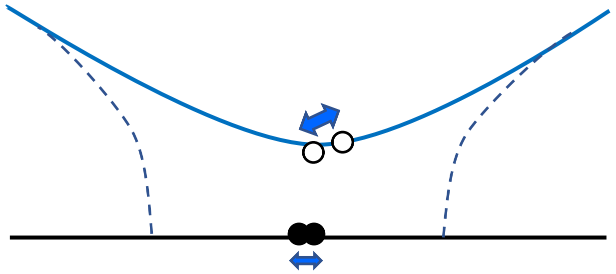


High-energy mode

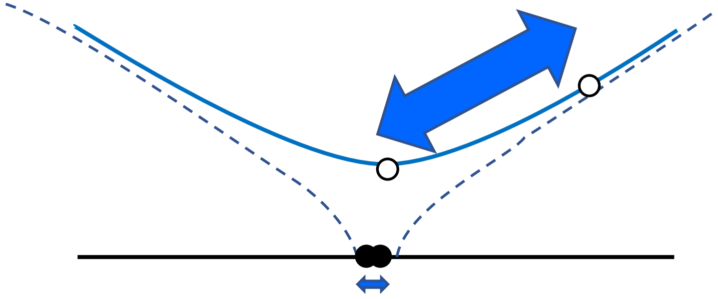


Flowed pt. going away…

Otherwise,



Strong autocorrelation



1. Introduction

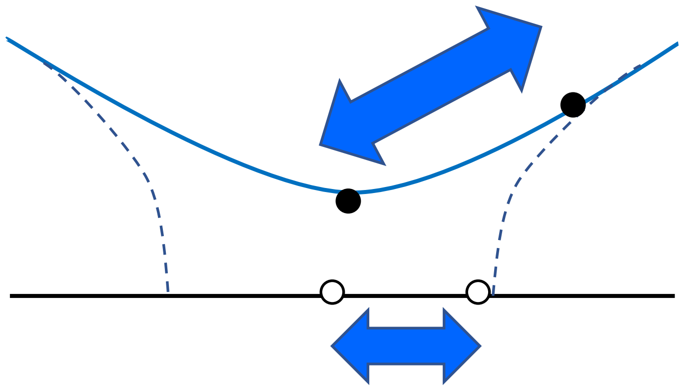
Then, when we take the sampling with multimode…

Case b) Sampling point on the deformed contour [Fukuma-Matsumoto, ’20]

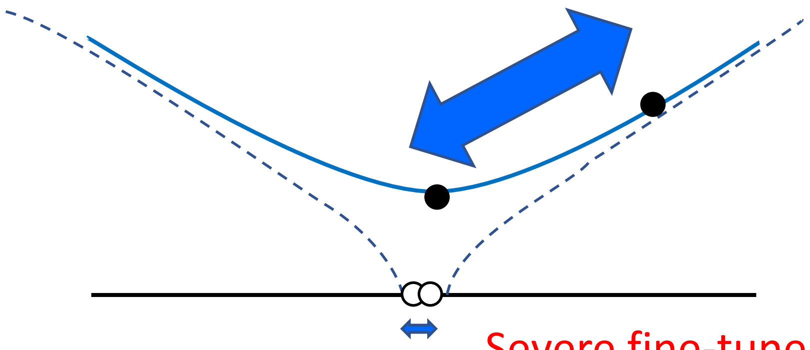
Cf) [Fujii-Honda-Kato-Kikukawa-Komatsu-Sano, ’13]

Note: a reference point and its update are required to compute the sampling pt.

Low-energy mode



High-energy mode



Severe fine-tune of updates for reference pt.

2. Optimizing the flow

- Express the singular values of $\overline{H}$ as $\lambda_1 < \lambda_2 < \cdots < \lambda_N$

  The problematic hierarchy of the expansion modes is characterized by

$$\eta(\overline{H}) \equiv \frac{\lambda_N}{\lambda_1}$$

Condition number (linear equation) or Stiffness ratio (differential equation)

- In local theories, large η appears mainly due to the derivative in the kinetic term
- Typically, $\eta(\bar{H}) = O(1000)$ even with $N = O(10)$ → Averaging the flow time (at least) in Case a) is not so effective.

- In order to make the subtlety milder,

  A) improve the numerical algorithm so that we can go with large η

  B) modify the flow eq. to make η close to 1 ⟵ **Our work**

2. Optimizing the flow

Modified flow eq.

$$\frac{\partial z_j}{\partial \sigma} = A_{jk} \overline{\frac{\partial S}{\partial z_k}}, \qquad A_{jk}(z, \bar{z})$$: hermitian, positive-definite

"preconditioner"

- The essential property of the original flow eq. is inherited: $\frac{\partial S}{\partial \sigma} = \frac{\partial S}{\partial z_j} A_{jk} \overline{\frac{\partial S}{\partial z_k}} > 0$
- Flow eq. for deviation : $\frac{\partial(\delta z_j)}{\partial \sigma} = A_{jk}\overline{H_{kl}\delta z_l} \quad +(\partial_l A_{jk})\overline{\partial_k S}\delta z_l + c.c.$

  From interaction; small contribution to η in local theories

  ➡ Not $\eta(\overline{H})$ but $\eta(A\overline{H})$ matters!

We can freely choose $A_{jk}(z, \bar{z})$, but for the present purpose, it should be

- making $\eta(A\overline{H})$ as small as possible
- calculable at small cost

Trade-off

2. Optimizing the flow

One choice: full optimization as to η

$$A = (\overline{H}H)^{-\frac{1}{2}} \quad \Rightarrow \quad \eta(A\overline{H}) = 1$$

Full preconditioner

Proof)

Polar decomposition: $\overline{H} = KU$ (K : Hermitian, positive-semidefinite U : unitary)

$$\rightarrow \overline{H}H = H^{\dagger}H = K^2, \quad A = K^{-1}, \quad \eta(A\overline{H}) = \eta(U) = 1$$

We have had a simulation with this choice for Case a),
And investigated basic properties

Sampling pt. on the original contour

3. Result with full preconditioner

Set up

- Model: wavefunction of an anharmonic oscillator with Gaussian initial state

$$\psi_{\rm fin}(b) = \int^{x(T)=b} \mathcal{D}x\, e^{-S} \psi_{\rm ini}(x(0))$$

$$S = -i \int dt \left(\frac{\dot{x}^2}{2} - \frac{\lambda}{4!} x^4 \right), \quad \psi_{\rm in}(x) = const. \times \exp\left(-\frac{\gamma}{4}(x-a)^2 \right)$$

$T = (N+1)\epsilon$

$$\psi_{\rm fin}(b) = \int dx_1 \cdots dx_N\, e^{-S}$$

$$S = -i \sum_{i=0}^{N} \epsilon \left(\frac{(x_{i+1}-x_i)^2}{2\epsilon^2} - \frac{\lambda}{4!} \frac{x_{i+1}^4 + x_i^4}{2} \right) + \frac{\gamma}{4}(x_0 - a)^2, \quad x_{N+1} = b$$

- To move the sampling pt., we employ the backpropagating Hybrid Monte-Carlo

[Fujisawa-Nishimura-KS-Yosprakob, ’21]

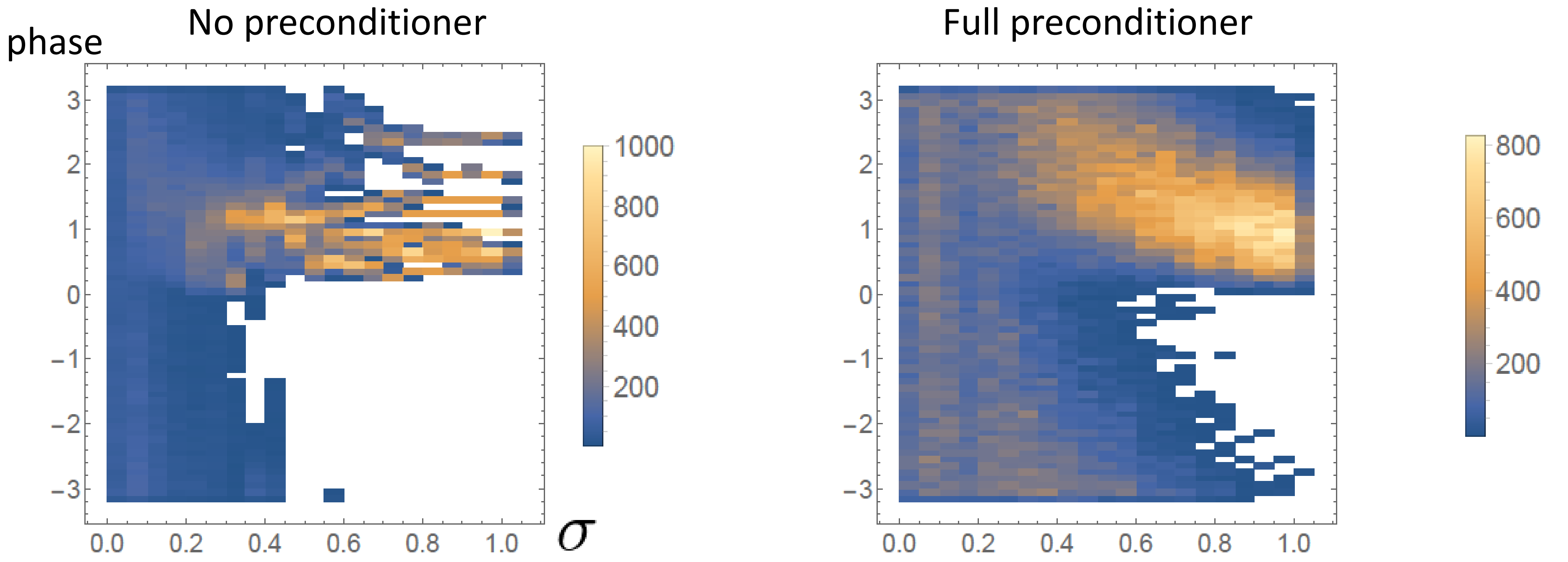
HMC …… Update sampling pt. to distant place by “rolling down” the point with potential *S*.
Backpropagation …… Fast calculation of the “force” to move the point for Case a); we solve the flow eq. backwardly.

3. Result with full preconditioner

Distribution of phase factor $e^{-i\mathrm{Im}\,S}$

$$N=6, T=2, \gamma=1,$$
$$a=1, b=0, \lambda=1.$$

50000 samples
for each



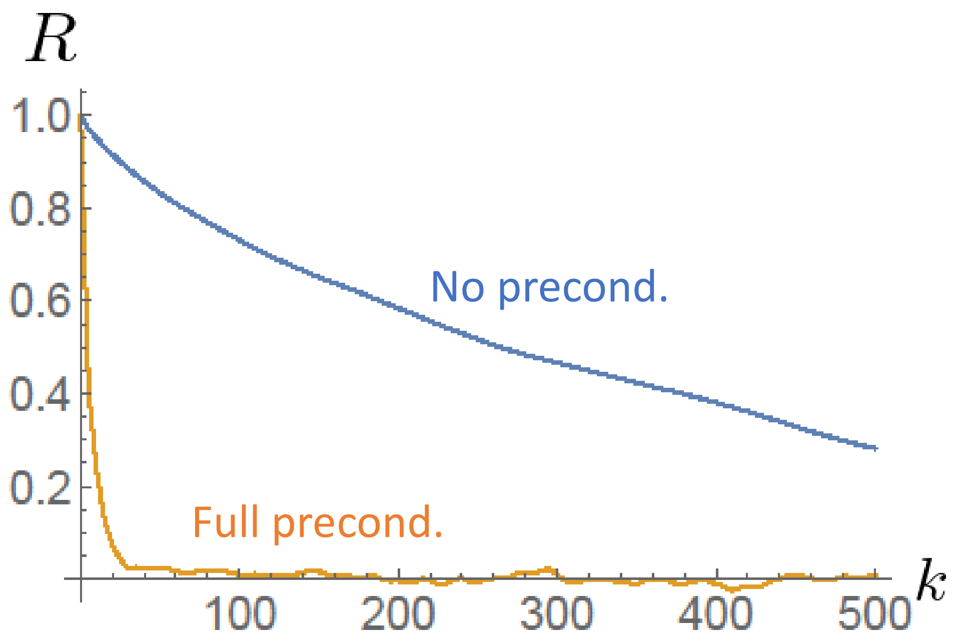
With the full preconditioner, we observed that the suitable regions of σ,
where the sign prob. & Ergodicity prob. are resolved, are regulated among all the modes.

3. Result with full preconditioner

Autocorrelation

Between the samplings $x^{(i)}$ and $x^{(i+k)}$, the autocorrelation is defined as

$$R(x;k) = \sum_{n=1}^{N-k} \frac{(x^n - \langle x \rangle) \cdot (x^{n+k} - \langle x \rangle)}{\langle x^2 \rangle - \langle x \rangle^2}$$



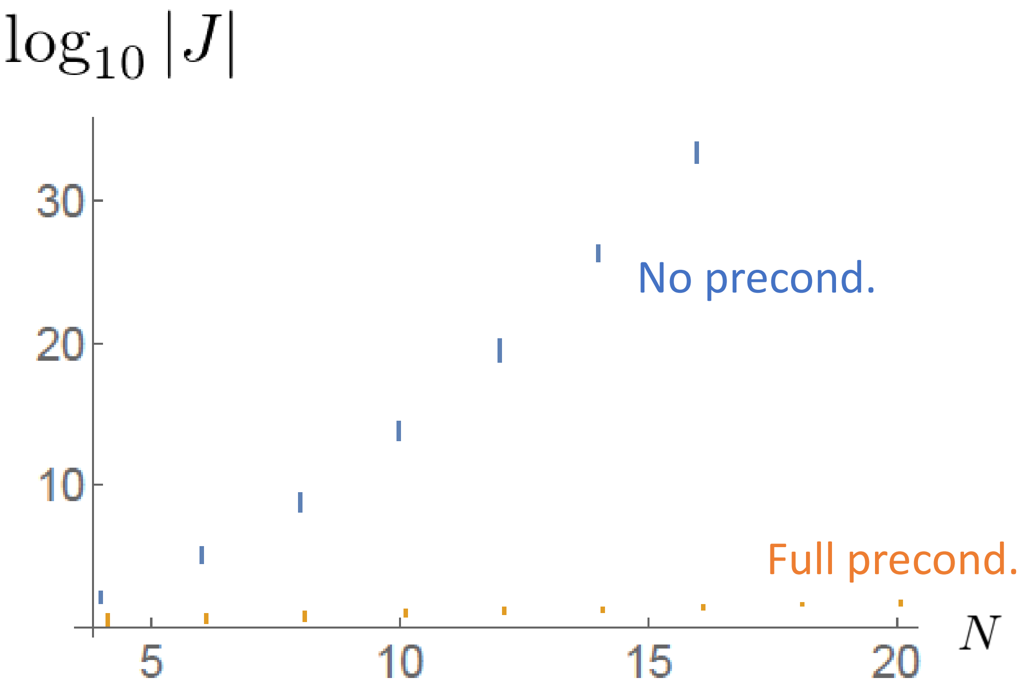
Satisfactory small autocorrelation!

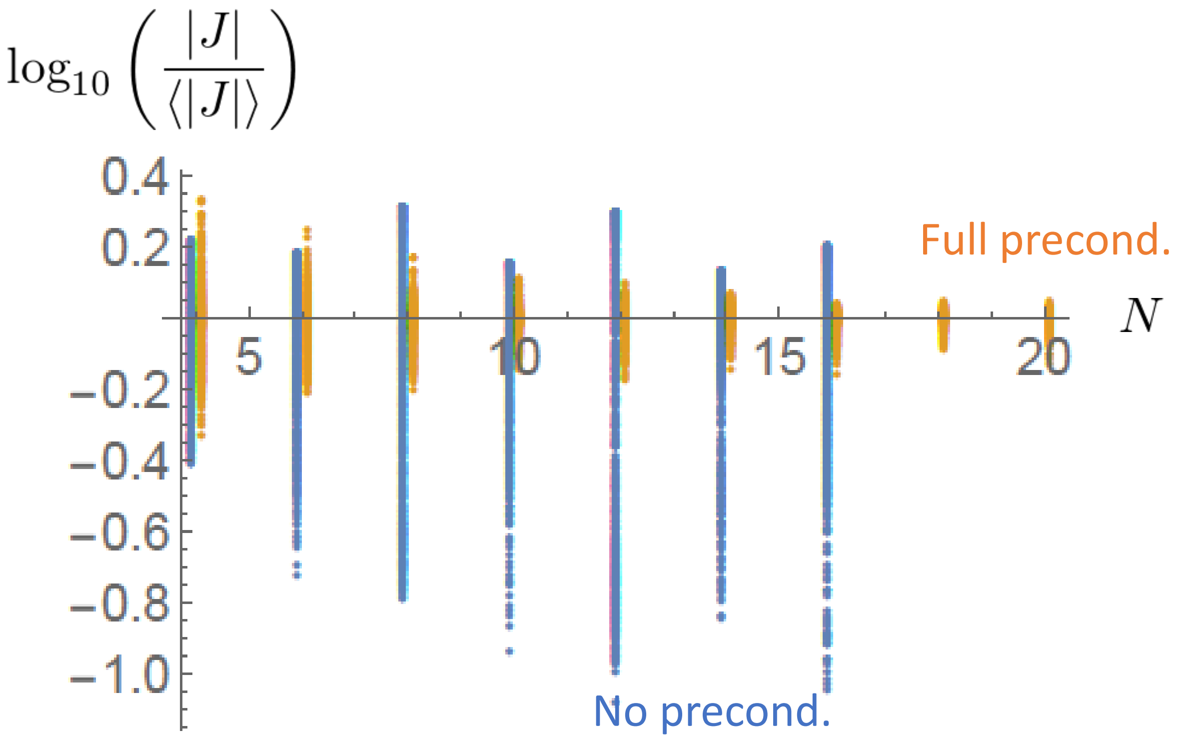
3. Result with full preconditioner

Fluctuation of Jacobian

In Case a), we have to include the Jacobian of the flow map in the observable.

→ tend to fluctuate by orders of magnitude, causing an overlap problem.





|J| gets less fluctuating

→ Overlap prob. is circumvented

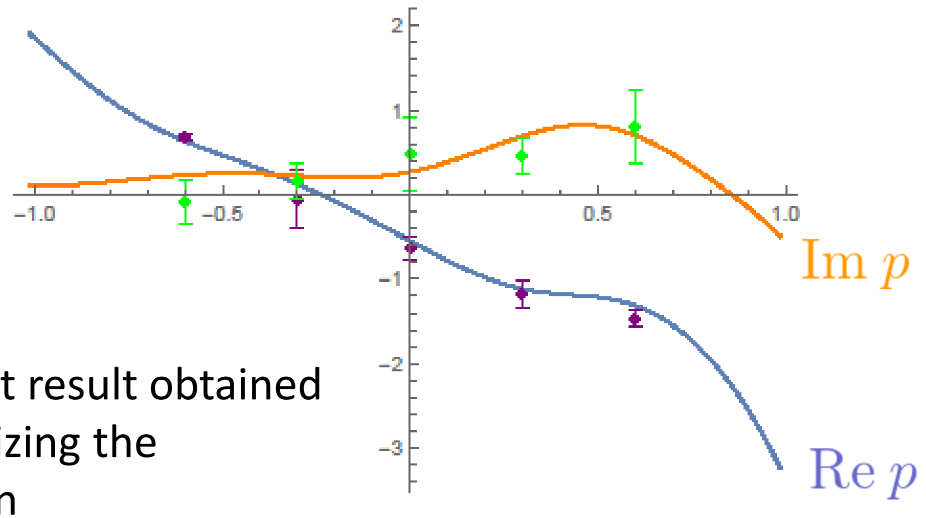
3. Result with full preconditioner

Larger system, stronger coupling (trial phase)

$$N = 20, \ \ \lambda = 30, \ \ \gamma = 4, \ \ a = 0.3$$

Observable: momentum density

$$p(b) = \partial_b (\log \psi_{\rm fin}(b)) \ = \frac{\partial_b \, \psi_{\rm fin}(b)}{\psi_{\rm fin}(b)} \qquad \langle P \rangle = \int db \, |\psi_{\rm fin}(b)|^2 \, p(b)$$



Curves: exact result obtained by diagonalizing the Hamiltonian

Without preconditioner, it's very hard to obtain a result with a same-order precision in a realistic running time.

↓

The applicability of GTM is enlarged, indeed!

4. Summary and Future works

Summary

- We have discussed a subtlety in standard flow eq. in GTM, which comes from the hierarchy in the expansion rates. This is more crucial when we move the sampling pt. on the original contour.

- We have proposed a modification on the flow eq. by a preconditioner, which reduces the higherarchy.

- We have demonstrated a simulation for a real-time anharmonic oscillator, and have confirmed regulated suitable region of flowtime, small autocorrelation, small fluctuation of the Jacobian, enlarged applicability of GTM.

Future works

- Improvement on Case b), where we move the sampling pt. on the deformed contour?

Constraint eq. for updating parameters

$$\frac{\partial f_j}{\partial \epsilon_k}\delta\epsilon_k + \frac{\partial f_j}{\partial \lambda^a}\delta\lambda^a = -f_j,$$

Reference pt.s

Multiplier

Normal force

$$f_j(\epsilon, \lambda) \equiv z_j(x+\epsilon, \sigma) - z_j(x, \sigma) - p_j \Delta s - \lambda^a F_j^a$$

Eq. with huge condition number → reduced by a preconditioner

Or, world volume method [Fukuma-Matsumoto, '21, …] (Prof. Fukuma's talk) with large-cond.num.-tolerant algorism?

- Other choices of the preconditioners, faster at the cost of η≠1 ?

- physical application such as quantum tunneling (Dr. Yosprakob's talk), quantum cosmology (Prof. Nishimura's talk)

Listen to them tomorrow!

Back up

1. Introduction

Why expansive map?

- flow eq. for deviation $\delta z_j = z_j - z'_j$: $\frac{\partial(\delta z_j)}{\partial\sigma} = \overline{H}_{jk}\overline{\delta z_k}$ Hessian

➡ Roughly, exponential expansion with rates "singular values of $\overline{H}$"

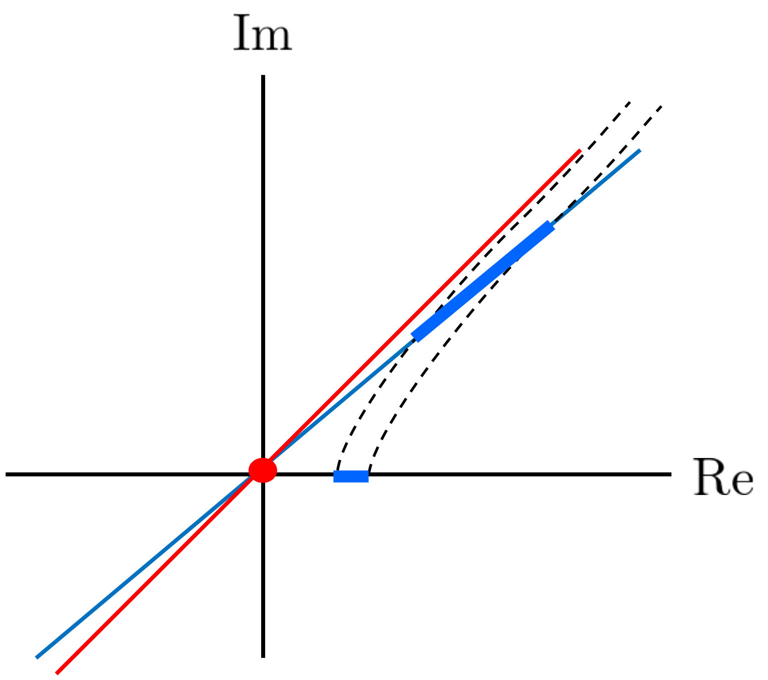
Ex) Real time free particle $S = -i\int dt\,\frac{\dot{x}(t)^2}{2}$

$$\frac{\partial z(t;\sigma)}{\partial\sigma} = i\frac{\partial^2\overline{z}(t;\sigma)}{\partial t^2}$$

Changing the variables: $z = x + iy,\ \ u = x + y,\ \ v = x - y$

$$\frac{\partial u}{\partial\sigma} = \frac{\partial^2 u}{\partial t^2}, \qquad \frac{\partial v}{\partial\sigma} = -\frac{\partial^2 v}{\partial t^2},$$

Time-reversal diffusion eq.



Cf) Turok, "Existence of real time quantum path integrals" ('22)