Unification of the complex Langevin method and the Lefschetz thimble method

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Parallel talk at LATTICE2017

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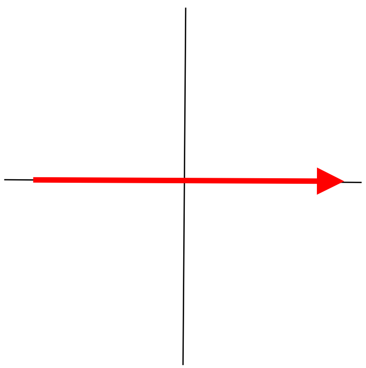
Ref.) J.N.-Shimasaki, JHEP06(2017)023 (arXiv:1703.09409 [hep-lat])

A new development toward solution to the sign problem 2011～

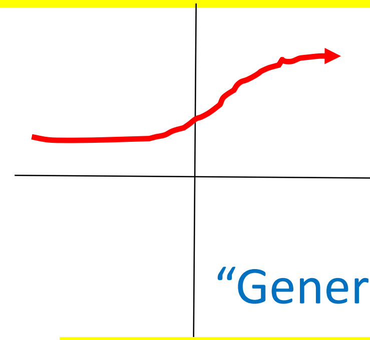
Key : complexification of dynamical variables

The original path integral

$$Z = \int dx\, w(x)$$



The phase of $w(x)$ oscillates violently (sign problem)

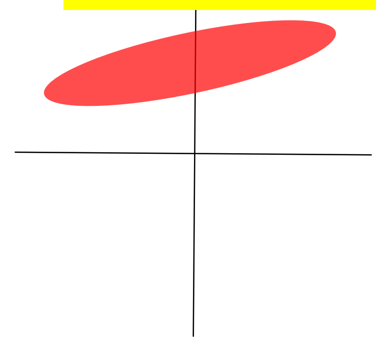


$$Z = \int dz\, w(z)$$

Minimize the sign problem by deforming the integration contour

“Generalized Lefschetz Thimble Method”

In this talk, we consider a unified formulation, which clarifies the relationship between the two.



An equivalent stochastic process of the complexified variables (no sign problem !)

“Complex Langevin Method”

The equivalence to the original path integral holds under certain conditions.

Plan of the talk

1. Brief review of CLM and GLTM
2. Unifying CLM and GLTM
3. Results for a single-variable model
4. Summary

1.Brief review of CLM and GLTM

We consider a general model defined by a multi-variable integral

$$Z = \int_{\mathbb{R}^n} dx \, e^{-S(x)}$$

$$x = (x_1, \cdots, x_n) \in \mathbb{R}^n$$

$$S(x) \in \mathbb{C}$$

$$\langle \mathcal{O}(x) \rangle = \frac{1}{Z} \int_{\mathbb{R}^n} dx \, \mathcal{O}(x) \, e^{-S(x)}$$

Difficult to evaluate due to the sign problem.

The complex Langevin method (CLM)

Parisi ('83), Klauder ('84)

$$x \to z = x + iy \in \mathbb{C}^n$$

$$\frac{\partial}{\partial t} z_k(t) = -\frac{\partial S(z)}{\partial z_k} + \eta_k(t)$$

real Gaussian noise

$$\langle \eta_k(t) \eta_l(t') \rangle_\eta = 2\,\delta_{kl}\,\delta(t-t')$$

holomorphically extended to functions of z

$$\langle \mathcal{O}(x) \rangle = \langle \mathcal{O}(z) \rangle_{\text{CLM}}$$

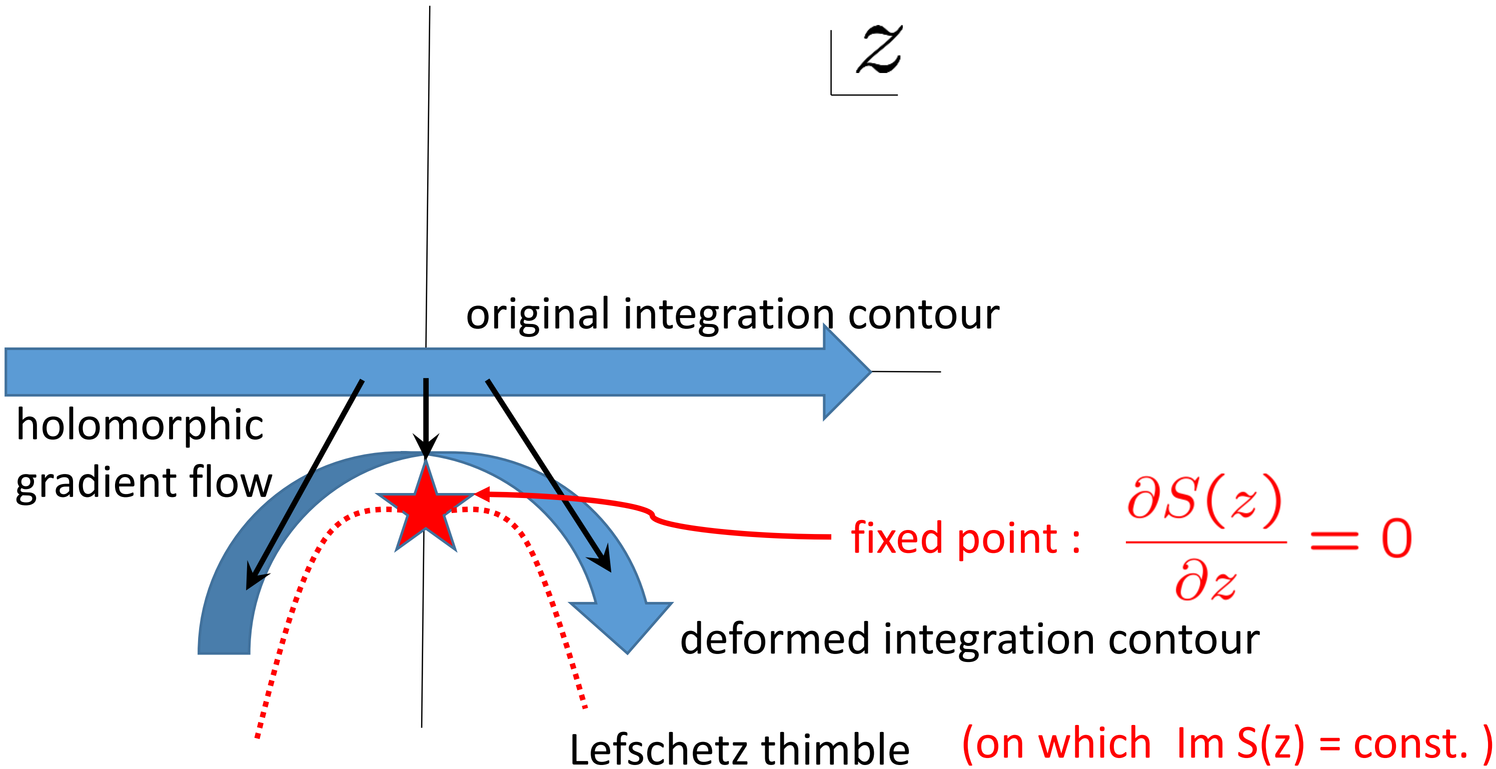
Under certain condition

G.Aarts, E.Seiler, I-O.Stamatescu, PRD81 (2010) 054508
K.Nagata, J.Nishimura, S.Shimasaki, PRD94 (2016) 114515

When the action S is real, this reduces to the (real) Langevin method (RLM), which is one of ordinary MC algorithms.

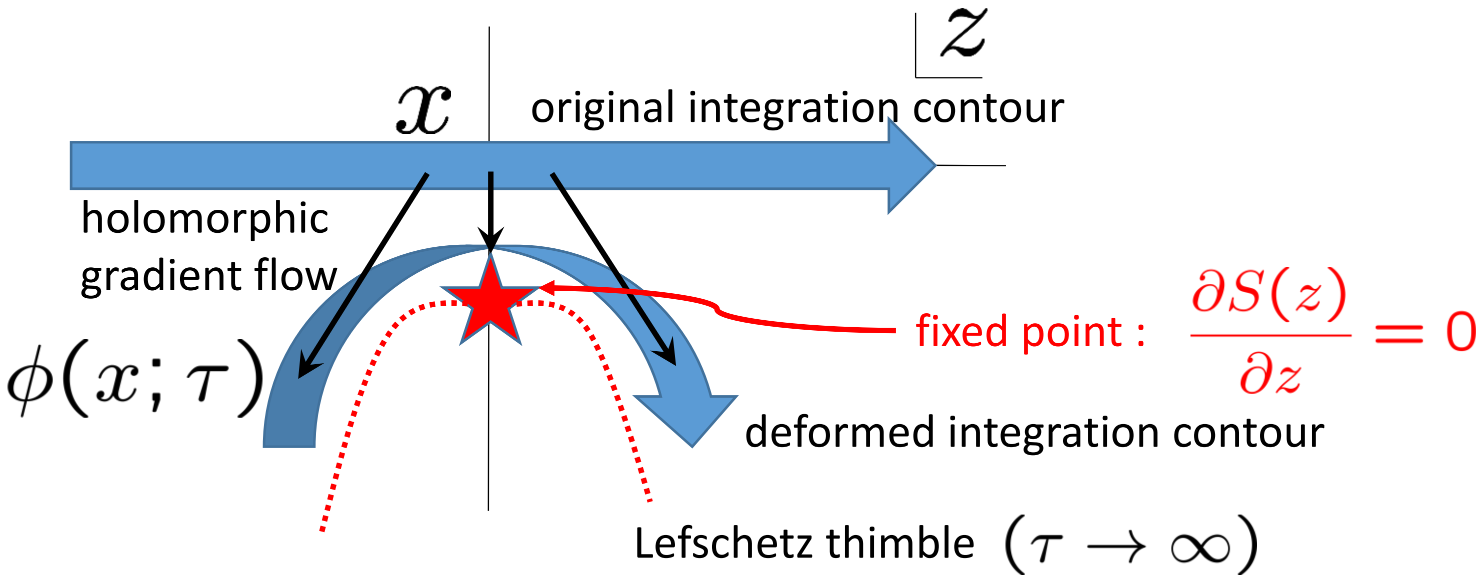
The generalized Lefschetz thimble method (GLTM)

A.Alexandru, G.Basar, P.F.Bedaque, G.W.Ridgway and N.C.Warrington, JHEP 1605 (2016) 053



As a result of the property of the holomorphic gradient flow, the sign problem becomes milder on the deformed contour !

The holomorphic gradient flow



solve $\quad \frac{\partial}{\partial \sigma}\phi_k(x;\sigma) = \overline{\left(\frac{\partial S(\phi(x;\sigma))}{\partial \phi_k}\right)}$

from $\sigma = 0$ to $\sigma = \tau$

with the initial condition $\phi(x;0) = x \in \mathbb{R}^n$

One obtains a one-to-one map from x to $\phi(x;\tau)$

The deformed integration contour

$$M_\tau = \{\phi(x;\tau) | x \in \mathbb{R}^n\}$$

n-dimensional real manifold in $\mathbb{C}^n$

$$Z = \int_{\mathbb{R}^n} dx\, e^{-S(x)}$$

$$= \int_{M_\tau} d\phi\, e^{-S(\phi)}$$

$$= \int_{\mathbb{R}^n} dx\, \det J(x;\tau)\, e^{-S(\phi(x;\tau))}$$

$$= \int_{\mathbb{R}^n} dx\, e^{-S_{\text{eff}}(x;\tau)}$$

$$J_{kl}(x;\tau) \equiv \frac{\partial}{\partial x_l}\phi_k(x;\tau)$$

$$S_{\text{eff}}(x;\tau) \equiv S(\phi(x;\tau)) - \log\det J(x;\tau)$$

$\det J \in \mathbb{C}$ and finite τ cause the residual sign problem.

$$\langle \mathcal{O}(x) \rangle = \frac{\langle e^{-i\,\text{Im}S_{\text{eff}}(x;\tau)} \mathcal{O}(\phi(x;\tau)) \rangle_{\text{Re}S_{\text{eff}}}}{\langle e^{-i\,\text{Im}S_{\text{eff}}(x;\tau)} \rangle_{\text{Re}S_{\text{eff}}}}$$

(reweighting)

CLM v.s. GLTM

	CLM	GLTM
Sign problem	◎ completely solved	○ residual sign problem exists
Numerical cost	○ O(V) for system size V	△ $O(V^3)$ for system size V
Range of applicability	△ condition for justification	○ works quite generally

For further development, it is desirable to clarify the relationship.

2. Unifying CLM and GLTM

The main idea of our proposal

$$Z = \int_{\mathbb{R}^n} dx\, e^{-S(x)}$$
$$= \int_{\mathbb{R}^n} dx\, \det J(x;\tau)\, e^{-S(\phi(x;\tau))}$$
$$= \int_{\mathbb{R}^n} dx\, e^{-S_{\text{eff}}(x;\tau)}$$

$$S_{\text{eff}}(x;\tau) \equiv S(\phi(x;\tau)) - \log\det J(x;\tau)$$

We apply the CLM to this system.

$$x \to z = x + iy \in \mathbb{C}^n$$

$$\frac{\partial}{\partial t} z_k(t) = -\frac{\partial S_{\text{eff}}(z)}{\partial z_k} + \eta_k(t)$$

drift term

$$\langle \mathcal{O}(x) \rangle = \langle \mathcal{O}(\phi(z;\tau)) \rangle_{\text{CLM}}$$

Calculation of the drift term

$$S_{\text{eff}}(x;\tau) \equiv S(\phi(x;\tau)) - \log\det J(x;\tau)$$

For the original real variables x, the drift term is:

$$\frac{\partial S_{\text{eff}}(x;\tau)}{\partial x_k} = \frac{\partial S(\phi(x;\tau))}{\partial \phi_l} J_{lk}(x;\tau) - J^{-1}_{lm}(x;\tau) K_{mlk}(x;\tau)$$

$$K_{mlk}(x;\tau) \equiv \frac{\partial}{\partial x_k} J_{ml}(x;\tau)$$

We need to extend it holomorphically to functions of z = x + iy.

$$\frac{\partial}{\partial \sigma}\phi_k(x;\sigma) = \overline{\left(\frac{\partial S(\phi(x;\sigma))}{\partial \phi_k}\right)} \qquad \phi_k(x;0) = x_k$$

⇩

$$\frac{\partial}{\partial \sigma}\phi_k(z;\sigma) = \overline{\left(\frac{\partial S(\phi(\bar{z};\sigma))}{\partial \phi_k}\right)} \qquad \phi_k(z;0) = z_k$$

Similarly for $J_{kl}(z;\sigma)$ and $K_{mlk}(z;\sigma)$.

3. Results for a single-variable model

Application of our unified formulation to a single-variable model

$$Z = \int dx\, (x+i\alpha)^p\, e^{-x^2/2}$$
$$= \int dx\, J(x;\tau)\, (\phi(x;\tau)+i\alpha)^p\, e^{-\phi(x;\tau)^2/2}$$

Sign problem occurs for $\alpha \neq 0$ and $p \neq 0$.

Here, $p=4$, $\alpha=4.2$.

J.Nishimura, S.Shimasaki , PRD92 (2015) 011501

We consider 3 versions of our formulation :

(i) CLM applied to the full model $\langle \mathcal{O}(x) \rangle = \langle \mathcal{O}(\phi(z;\tau)) \rangle_{\text{CLM}}$

This version does not require reweighting as in the ordinary CLM.

(ii) CLM applied to the partially phase-quenched model $Z_{\text{pPQ}} = \int dx\, |J(x;\tau)|\, (\phi(x;\tau)+i\alpha)^p\, e^{-\phi(x;\tau)^2/2}$,

This interpolates ordinary CLM and Lefschetz thimble method.

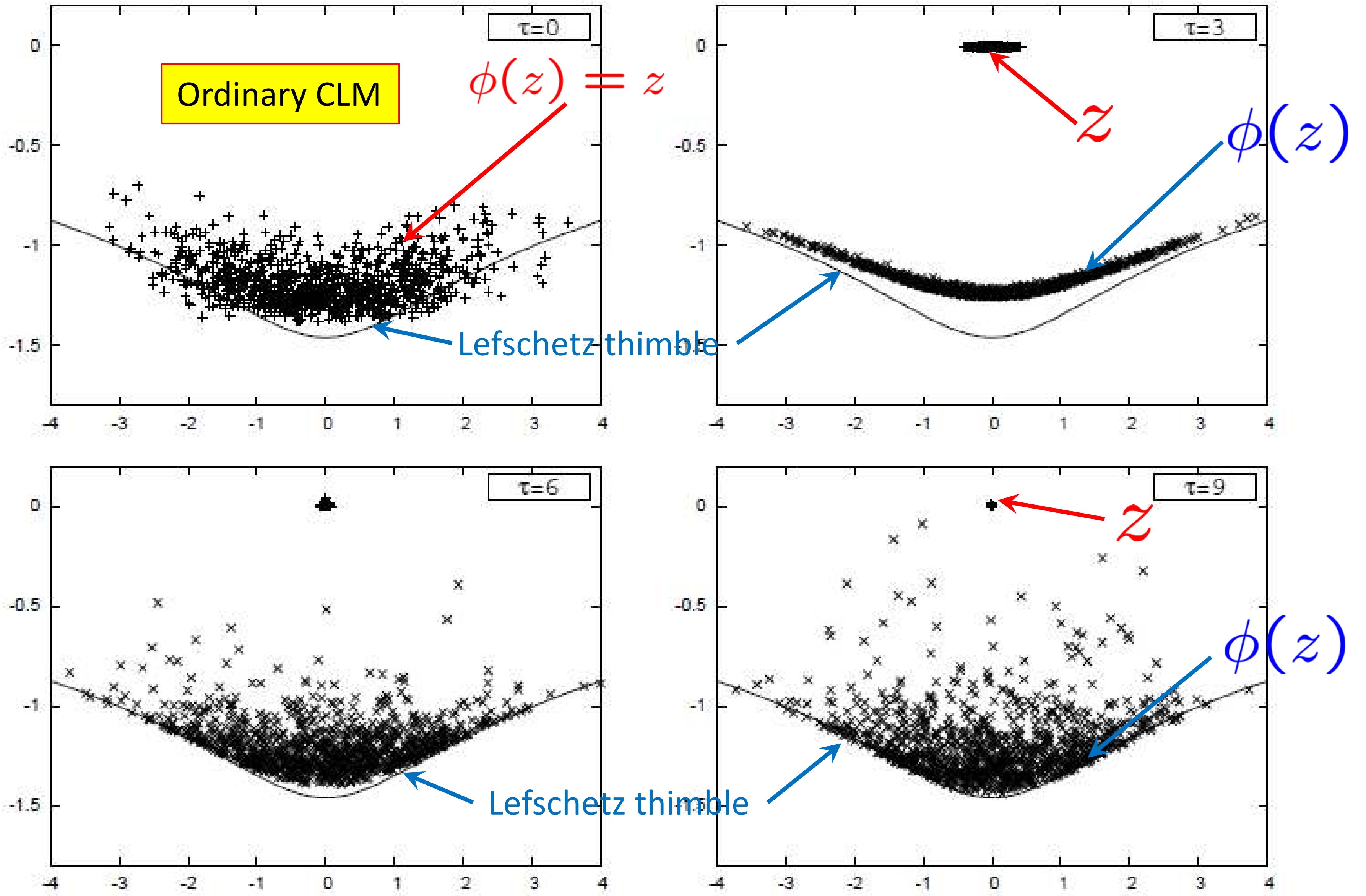
(iii) RLM applied to the totally phase-quenched model $Z_{\text{PQ}} = \int dx\, |J(x;\tau)\, (\phi(x;\tau)+i\alpha)^p\, e^{-\phi(x;\tau)^2/2}|$.

This is nothing but the GLTM using RLM for updating x.

Need reweighting in calculating EV. (applies to (ii) and (iii))

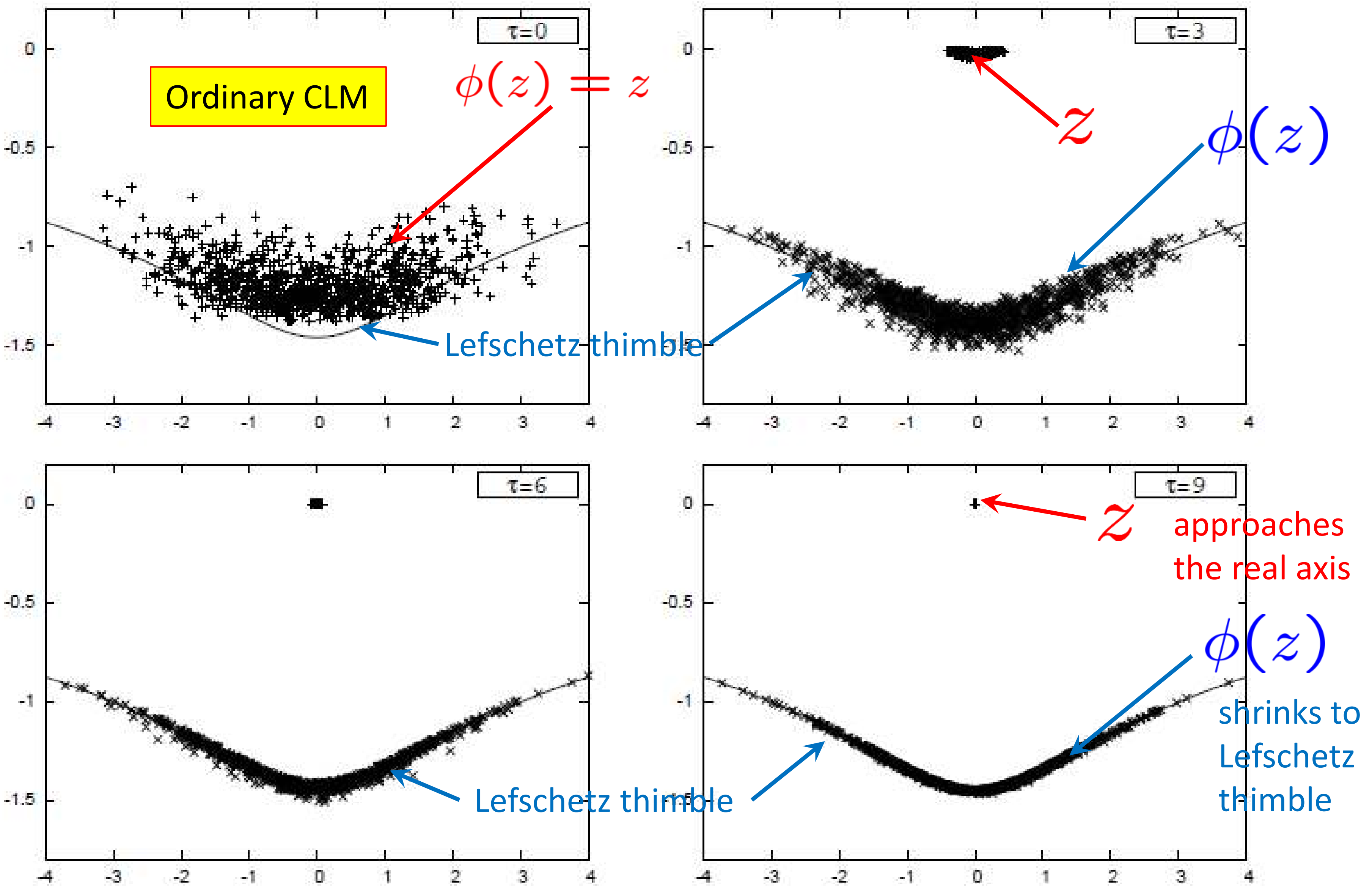
Results for the case (i)

The residual sign problem of the GLTM is taken care of by the complex Langevin dynamics.



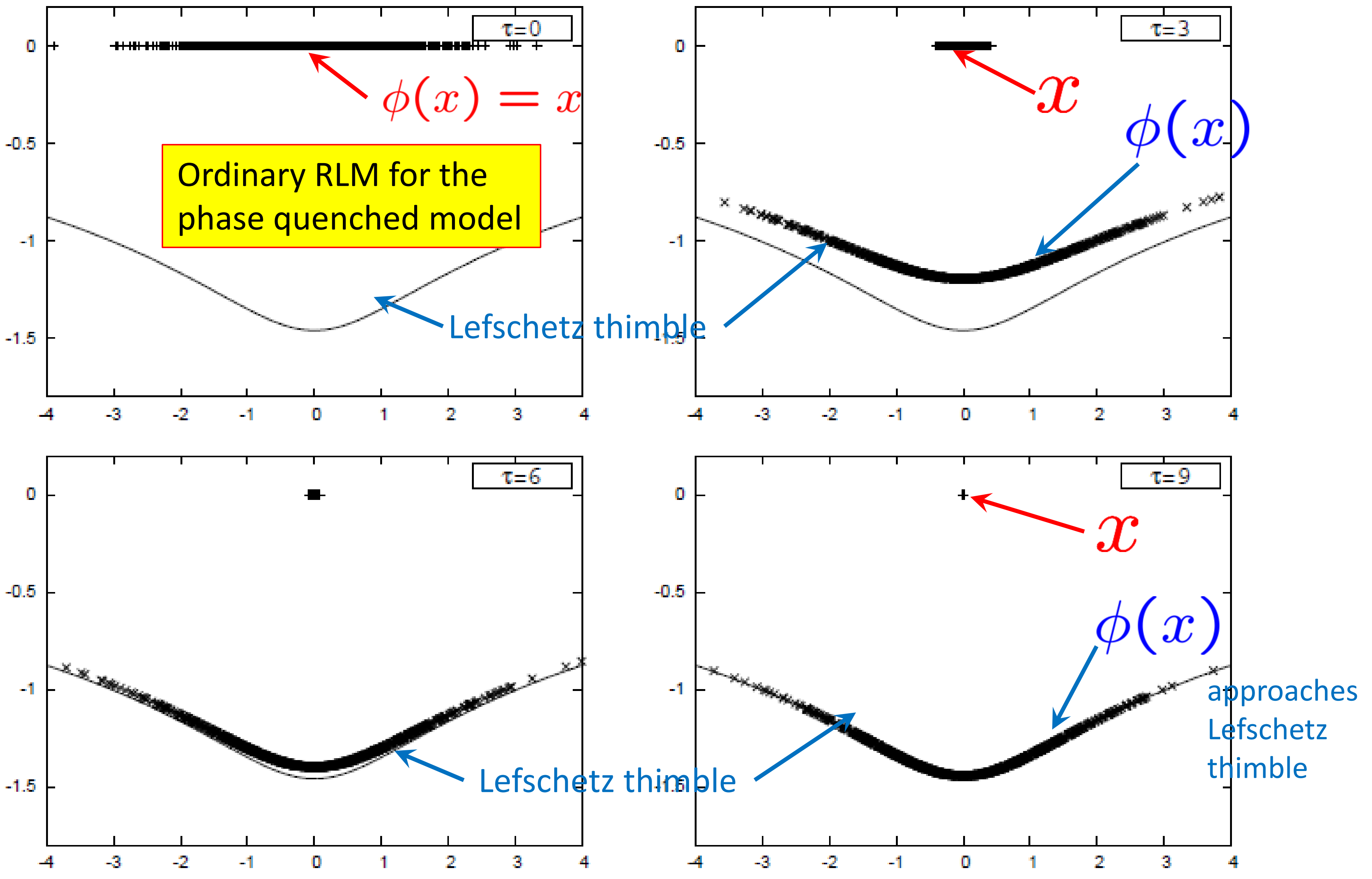
Results for the case (ii)

The residual sign problem due to Im S is taken care of by the complex Langevin dynamics.



Results for the case (iii)

The residual sign problem is taken care of by reweighting. (as in ordinary GLTM)



4. Summary

Summary

Remarkable progress in two closely-related approaches to the sign problem :

- Complex Langevin Method (CLM)
- Generalized Lefschetz Thimble Method (GLTM)

both based on <u>complexification of the dynamical variables</u>

The relationship between the two methods was not clear, though.

We have proposed a unified formulation :

(i) $$Z = \int_{\mathbb{R}^n} dx \, e^{-S(x)}$$

$$= \int_{\mathbb{R}^n} dx \, \det J(x;\tau) \, e^{-S(\phi(x;\tau))}$$

GLTM

We apply the CLM to this system.

$$\langle \mathcal{O}(x) \rangle = \langle \mathcal{O}(\phi(z;\tau)) \rangle_{\text{CLM}}$$

Summary (cont'd)

We also consider other versions such as applying CLM to :

(ii) $$Z_{\text{pPQ}} = \int_{\mathbb{R}^n} dx \, |\text{det} J(x;\tau)| \, e^{-S(\phi(x;\tau))}$$

(iii) $$Z_{\text{PQ}} = \int_{\mathbb{R}^n} dx \, \left|\text{det} J(x;\tau) \, e^{-S(\phi(x;\tau))}\right|$$

This case is nothing but the GLTM with RLM used for updating x.

In a single-variable model, we find that

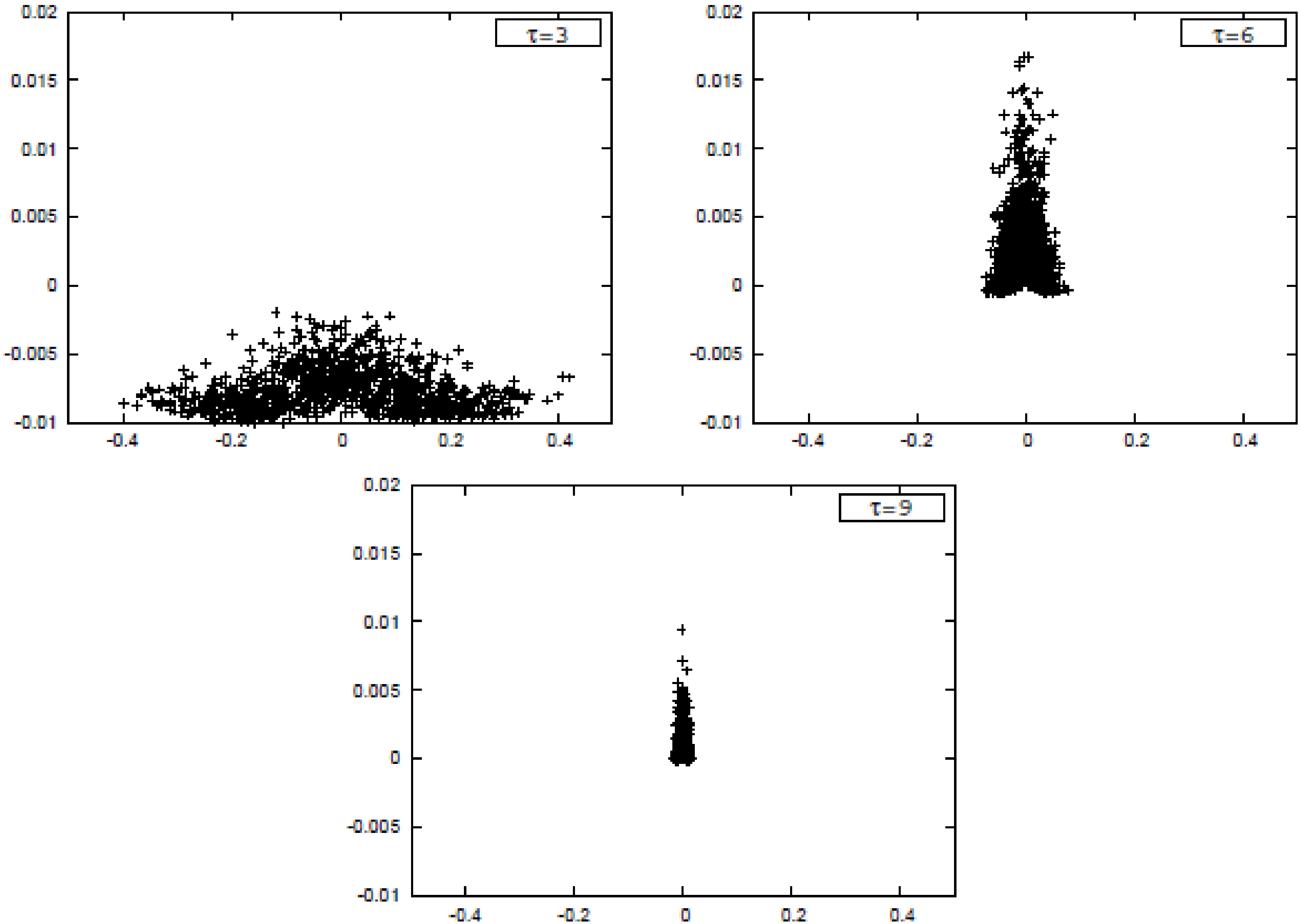
(ii) interpolates CLM ($\tau = 0$) and original Lefschetz thimble method ($\tau = \infty$).

Thus, our unified formulation provides a clear understanding on the relationship among CLM, GLTM, and the original Lefschetz thimble method.

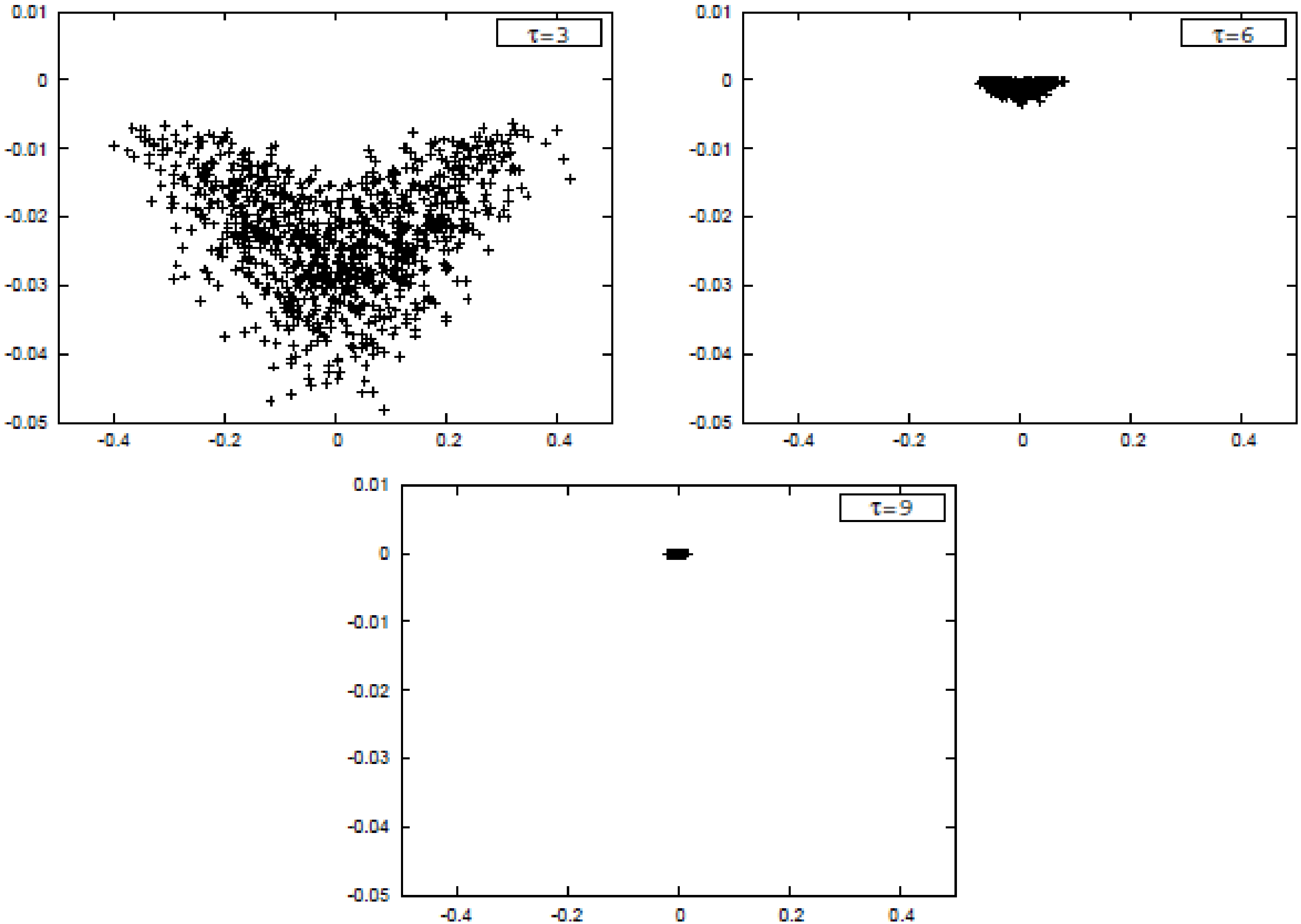
We hope this understanding will be useful in improving these methods further !

5. Backup slides

Zoom up of the distribution of z in the case (i)



Zoom up of the distribution of z in the case (ii)



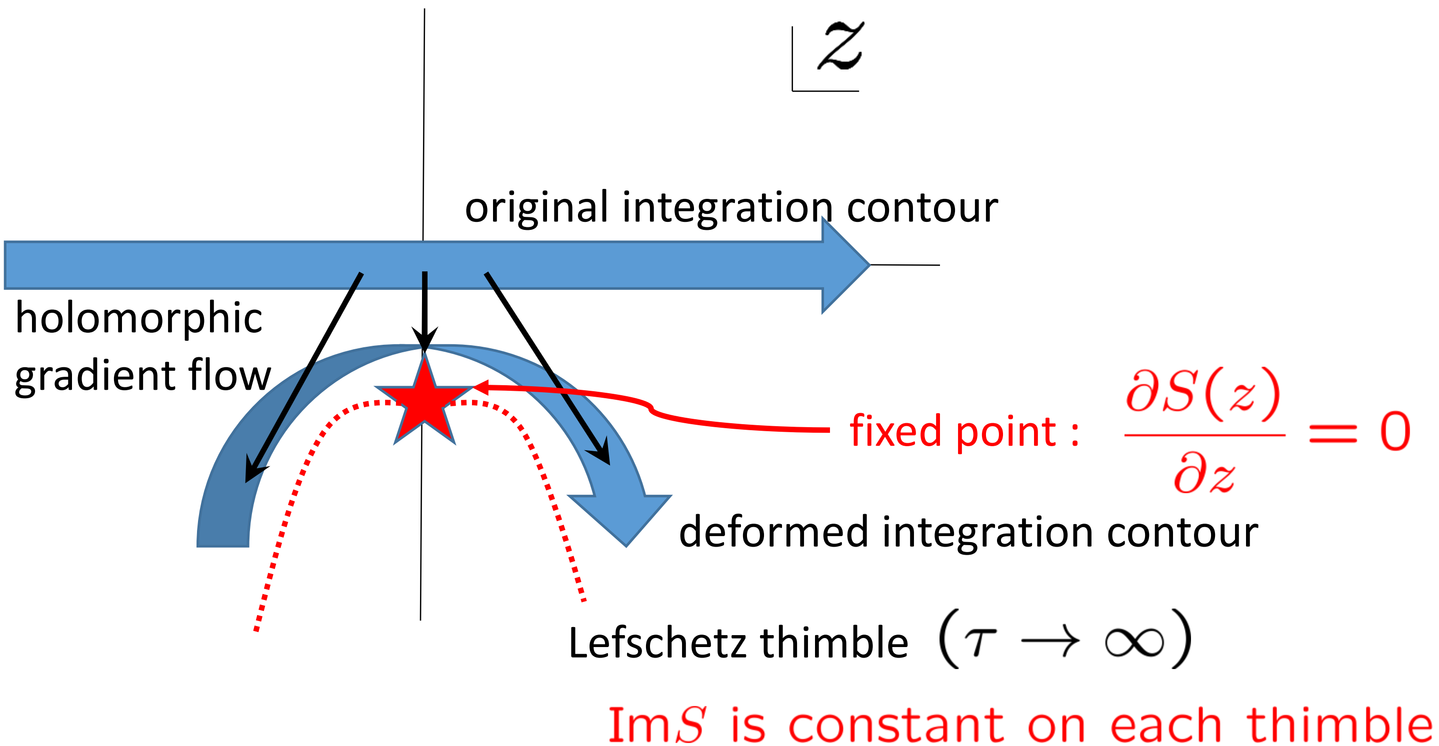
An important property of the holomorphic gradient flow

$$
\begin{aligned}
\frac{d}{d\sigma} S(\phi(x;\sigma)) &= \frac{\partial S(\phi(x;\sigma))}{\partial \phi_k} \frac{\partial \phi_k(x;\sigma)}{\partial \sigma} \\
&= \frac{\partial S(\phi(x;\sigma))}{\partial \phi_k} \overline{\left(\frac{\partial S(\phi(x;\sigma))}{\partial \phi_k} \right)} \\
&= \left| \frac{\partial S(\phi(x;\sigma))}{\partial \phi_k} \right|^2
\end{aligned}
$$

real positive !

Real part of the action increases along the flow, while the imaginary part is kept constant.

The integration is dominated by a small region of x as the flow-time increases.



As a result, the sign problem becomes milder !

The flow-time should not be too large when there exist more than one thimbles in order to avoid the ergodicity problem.