# *optimization*
# *Path ~~modification~~ method for the sign problem*

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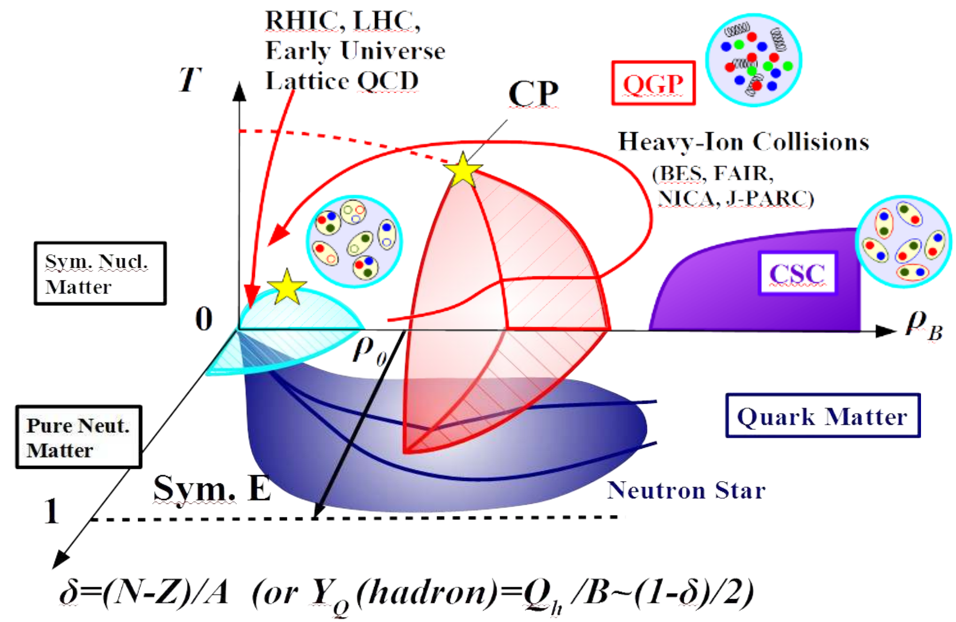
Lattice2017

*Y. Mori, K. Kashiwa, A. Ohnishi, arXiv:1705.05605*

# Introduction

- **Sign problem for complex actions**
  - **Grand challenge in theor. phys.**
  - **Largest obstacle to explore QCD phase diagram**

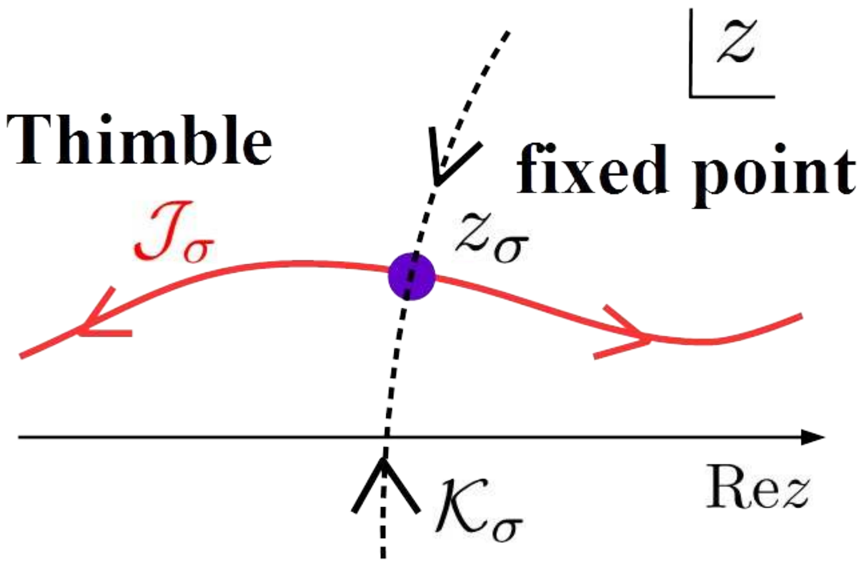



- **Approaches**
  - **Taylor expansion, Analytic cont., Canonical, Strong coupling, …**
  - **Complex Langevin method (CLM)**
    *G. Parisi ('83), G. Aarts et al. ('10)*
  - **Lefschetz thimble method (LTM)**
    *E. Witten ('10), Cristoforetti et al. ('12), Fujii et al. ('13)*
  - **Generalized LTM (GLTM)**
    *A. Alexandru, et al., ('16)*

***Complexified variables & Shifting path (area)***

# Lefschetz Thimble Method

- **Integral over thimbles defined by the flow equation for complexified variables → Im S = const. on a thimble**




$$\mathcal{Z} = \int_{\mathcal{C}_\mathbb{R}} \mathcal{D}x e^{-S[x]} = \int_{\mathcal{C}} \mathcal{D}z e^{-S[z]}$$

$$\left.\frac{\partial S}{\partial z_i}\right|_{z_\sigma} = 0 \ , \quad \frac{dz_i(t)}{dt} = \overline{\left(\frac{\partial S[z]}{\partial z_i}\right)}$$

$$\mathcal{C} = \sum_\sigma n_\sigma \mathcal{J}_\sigma \ , \quad n_\sigma = \langle \mathcal{C}_\mathbb{R}, \mathcal{K}_\sigma \rangle$$

- **Cons**
  - **Phase from measure (residual sign prb.)**
  - **Cancellation between thimbles (global sign prb.)**
  - **Flow equation blows up somewhere.**

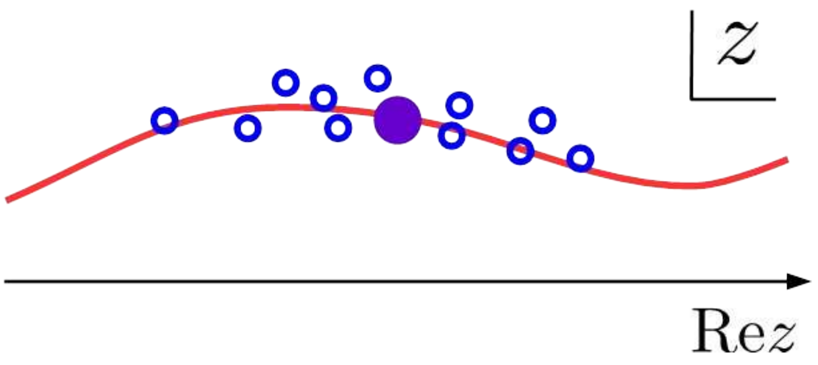
# Complex Langevin Method

- Sample configurations
  by solving complex Langevin equation
  for complexified variables.

$$\frac{dz_i}{dt} = -\frac{\partial S}{\partial z_i} + \eta(t)$$

$$\langle \eta_i(t)\eta_j(t)\rangle = 2\delta_{ij}\delta(t-t')$$

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




- Pros
  - Easier to apply to large DOF theories
- Cons
  - Excursion problem → Gauge Cooling *(Seiler et al. ('13))*
  - Converged results can be wrong → Criteria *(Nagata et al. ('16))*
  - Singular drift problem → Several prescriptions ….

***Is there any way to obtain the path without solving the flow equation and without suffering from singular points ?***

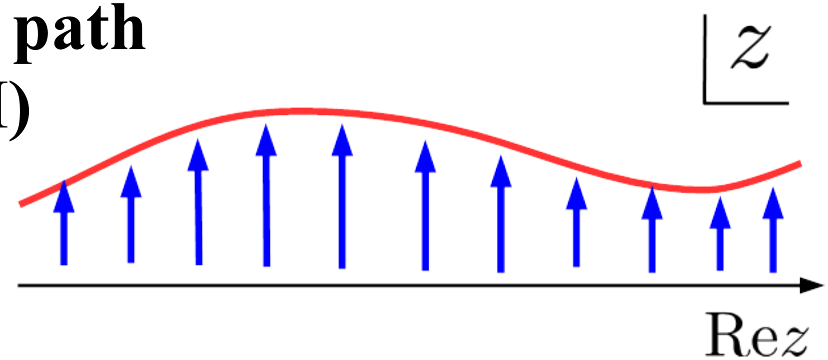
# *Contents*

- Introduction
- Path Optimization Method
- Application to a Toy Model
- Summary

# *Path Optimization Method*

# *Path Optimization Method*

- **Can we obtain the integration path without solving flow equation ?**
  **→ Variational shift of the integration path**
  **(Path Optimization Method: POM)**



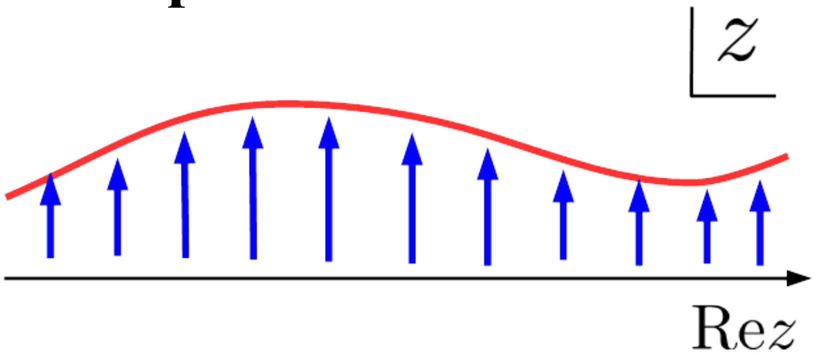

- **POM Procedure**
  - **Parametrize the path appropriately (Trial Function)**
  - **Set a measure of sign problem (Cost Function)**
  - **Tune parameters to minimize the Cost Function (Optimization)**

***Sign Problem → Optimization Problem***

# Trial Function, Cost Function, and Optimization

- **Parametrize the path in the complex plane (Trial Function)**
  - **Ex. one variable case → Expand in the complete set**

$$z(t) = x(t) + iy(t)$$
$$= t + \sum_n (c_n^{(x)} + ic_n^{(y)}) H_n(t)$$




$$\mathcal{Z} = \int dt J(t) e^{-S(z(t))}, \; J(t) = \frac{dz(t)}{dt}$$

- **Set the seriousness of the sign problem (Cost Function)**
  - **How much the phase fluctuate**

$$F[z(t)] = \frac{1}{2\mathcal{Z}} \int dt \left| e^{i\theta(t)} - e^{i\theta_0} \right|^2 \left| J(t) e^{-S[z(t)]} \right|$$
$$= \left| \langle e^{i\theta} \rangle_{\rm pq} \right|^{-1} - 1 \quad \left[ \theta = \arg(Je^{-S}), \; \theta_0 = \arg(\mathcal{Z}) \right]$$

- **Optimization: Gradient descent, Neural Network, …**

# *Application to a toy model*

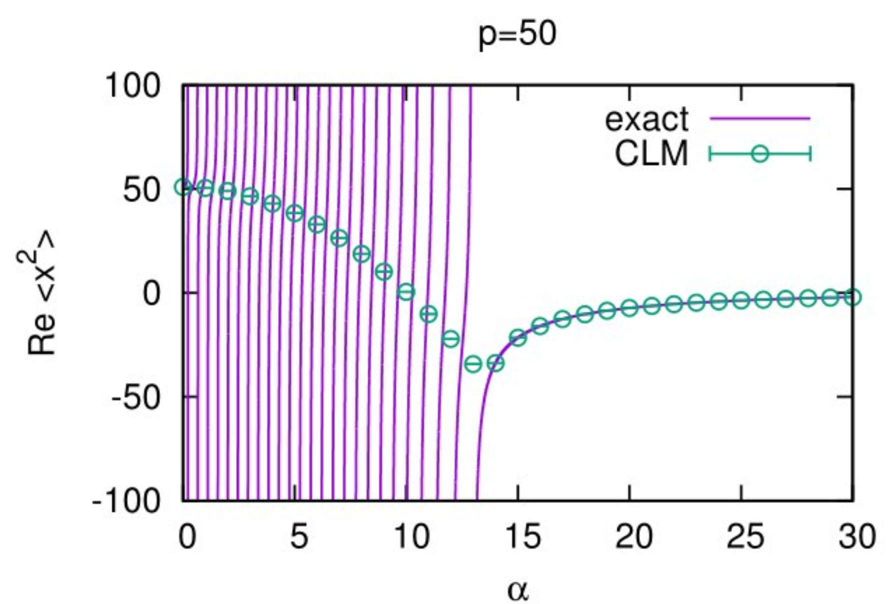
# *A (Pathological) Toy Model*

- **A toy model with a serious sign problem**
  *J. Nishimura, S. Shimasaki ('15)*

$$\mathcal{Z} = \int dx (x + i\alpha)^p \exp(-x^2/2) = \int dx \exp(-S)$$

$$S(x) = x^2/2 - p \log(x + i\alpha)$$

- **Complex Langevin Fails at Large *p* and small *α***
  - **Large p → Strong oscillation of the Boltzmann weight**
  - **Small α → Singular point at *z* = *-iα* is close to the real axis**



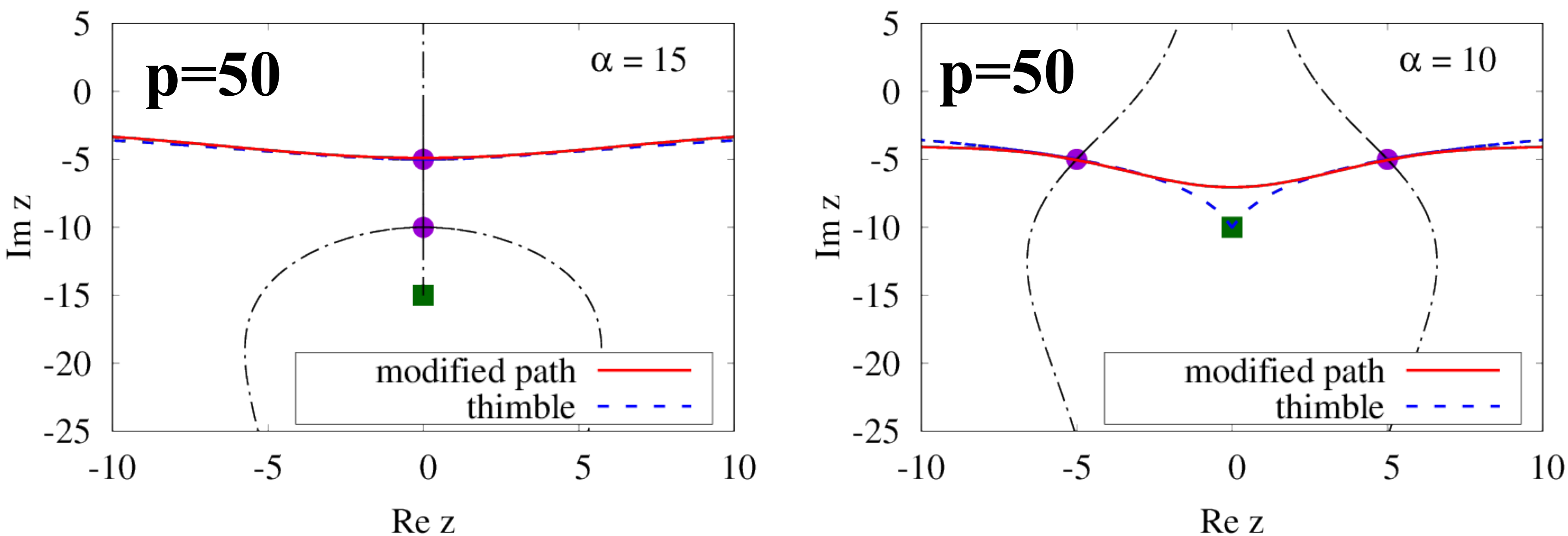
# Optimized Path

- **Trial Function**

*Mori, Kashiwa, AO ('17)*

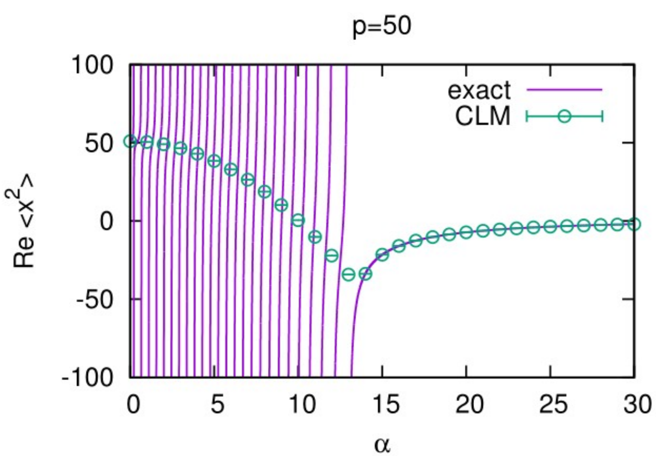
$$z(t) = t + i\left[c_1 \exp(-c_2^2 t^2/2) + c_3)\right]$$

- **Optimization = Gradient descent**
- **Optimized path agrees with thimble(s) around the fixed point(s) !**
  - **Large α → One thimble, Singular point is far away from thimble**
  - **Small α → Go through two FPs.**

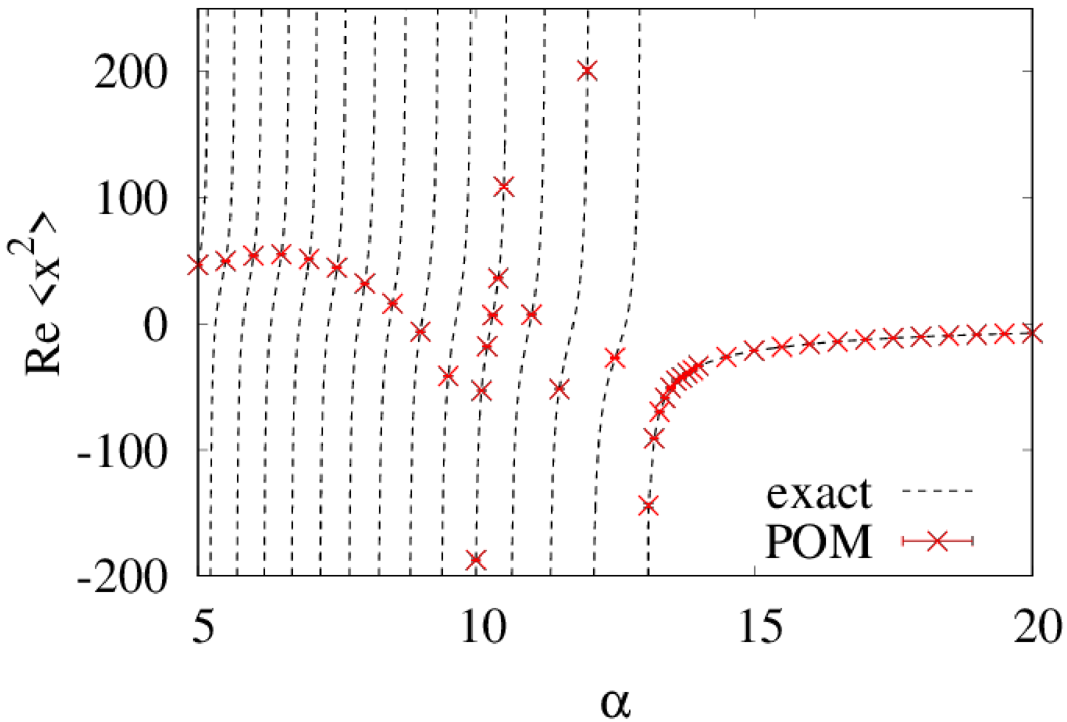


# *Expectation Value of $x^2$*

- **Hybrid MC results of $\langle x^2 \rangle$ on the optimized path well reproduce the exact results.**
- **Trick: ±x (=± Re(z)) gives same $|J\, e^{-S}|$ → Both ±x configurations are taken.**
- **Global sign prob. is not solved (and should not be solved).**



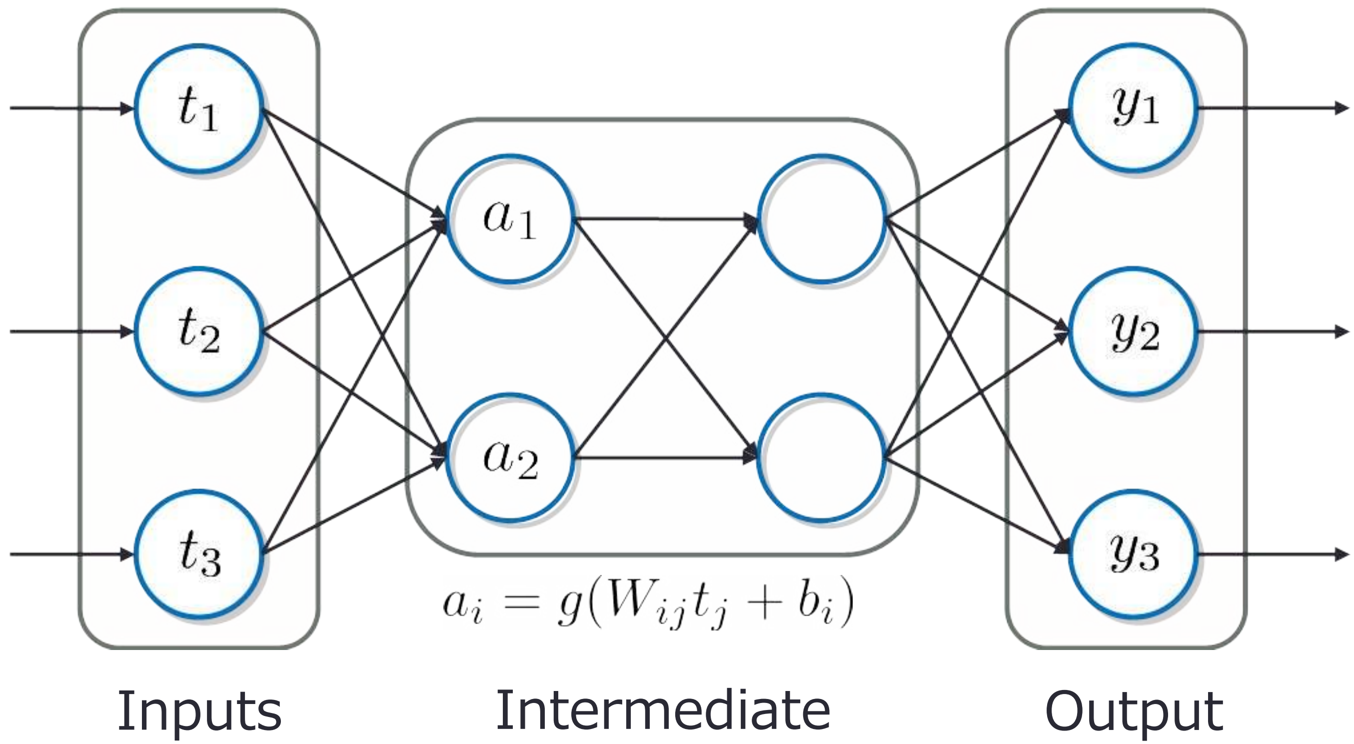

*Nishimura, Shimasaki ('15)*




*Mori, Kashiwa, AO ('17)*

# *Do we need to know the form of Trial Function ?*

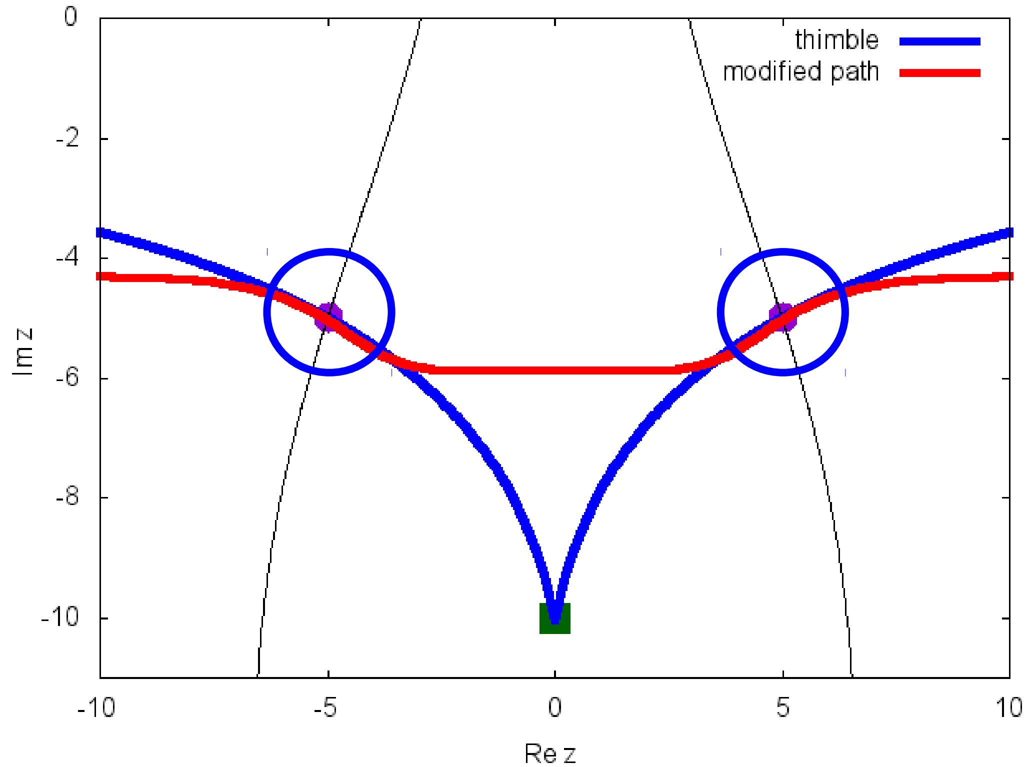
- **What happens for many variables ?**
  **Trial fn. form, Variable corr., CPU cost, …**
- **Neural Network**
  - **Combination of linear transf. + Non-linear network fn. g(x).**



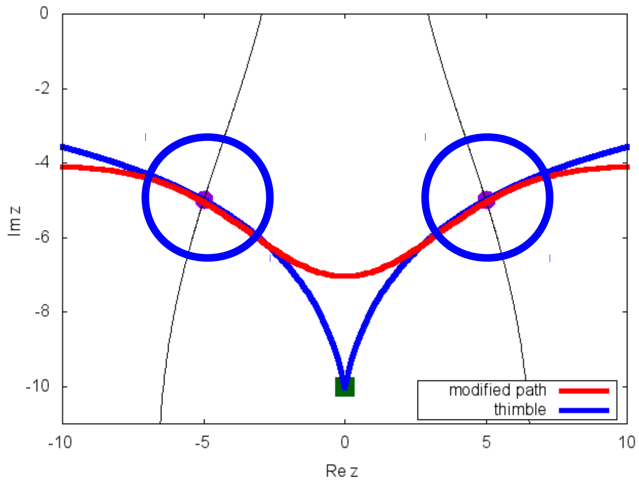

*Mori, Kashiwa, AO (in prep.)*

# Optimized Path by Neural Network

## Neural Network




## Gaussian +Gradient Descent



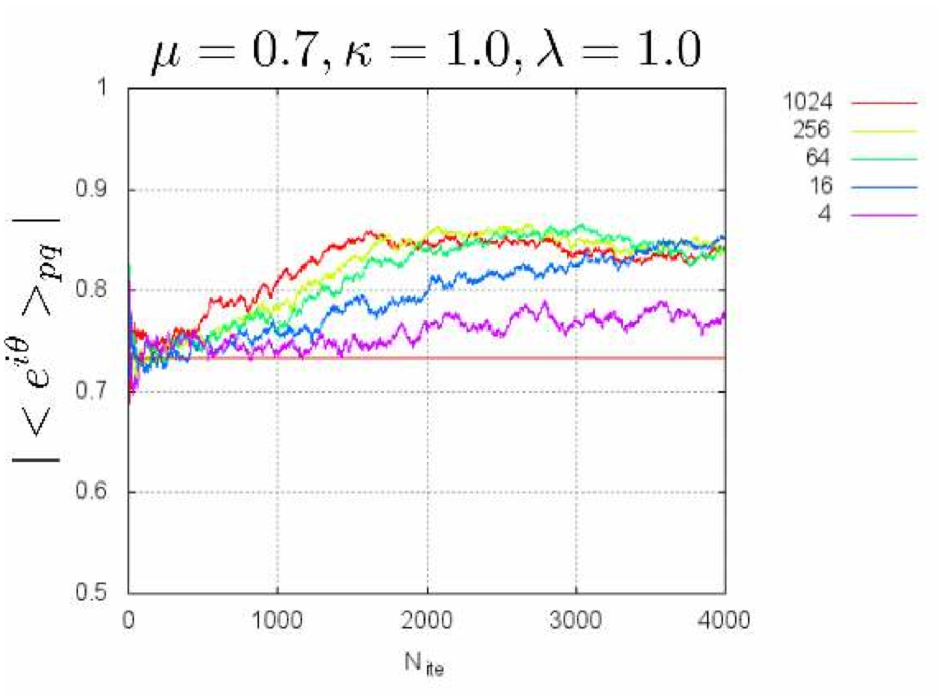

***Optimized paths are different,***
***but both reproduce thimbles around the fixed points !***

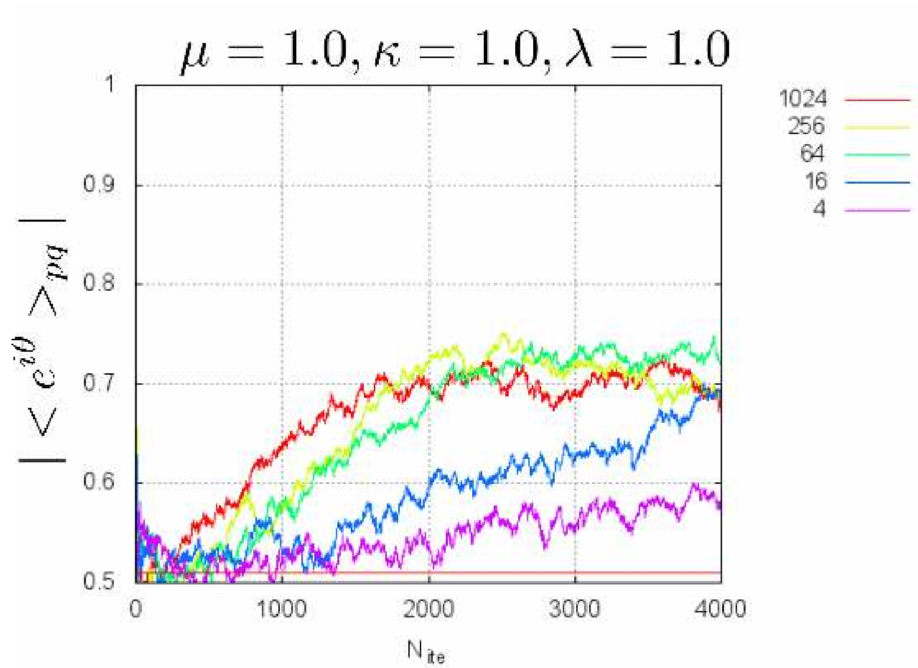
*Mori, Kashiwa, AO (in prep.)*

# Summary

- **Path Optimization Method is proposed to attack the sign problem.**
  - **Path is parametrized by the Trial Function.**
  - **Seriousness of the sign problem is given by the Cost Function.**
  - **Sign problem is regarded as the Optimization Problem.**
- **Usefulness of POM is demonstrated in a toy model.**
  - **Optimized path reproduces the thimble(s) around the fixed point(s).**
  - **Singular points with zero Boltzmann weight do not matter, since they do not contribute to the integral.**
  - **Global sign problem is unsolved (and should not be solved).**
- **It is possible to apply various optimization technique such as the neural network.**

## 4x4 lattice


$\mu = 0.7, \kappa = 1.0, \lambda = 1.0$
$| < e^{i\theta} >_{pq} |$
N ite
1024
256
64
16
4
1
0.9
0.8
0.7
0.6
0.5
0
1000
2000
3000
4000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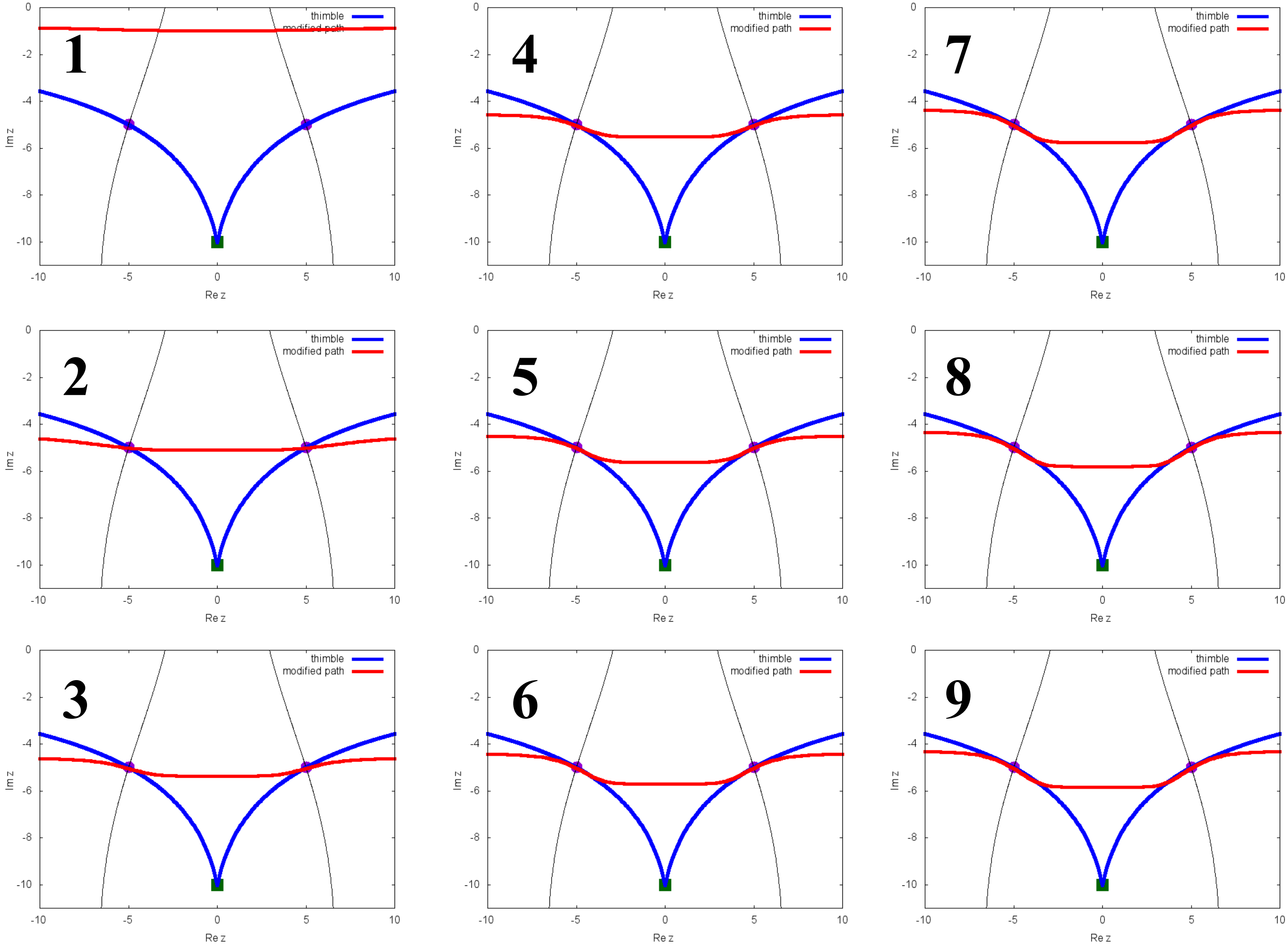
# *Optimized Path by Neural Network*



# Average Phase Factor

- **Boltzmann weight cancellation**
  - **Cancellation is mild at α > 14.**
  - **Weights at ±x strongly cancel with each other for α<14.**