# *Path optimization method to avoid the sign problem*

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**in collaboration with**
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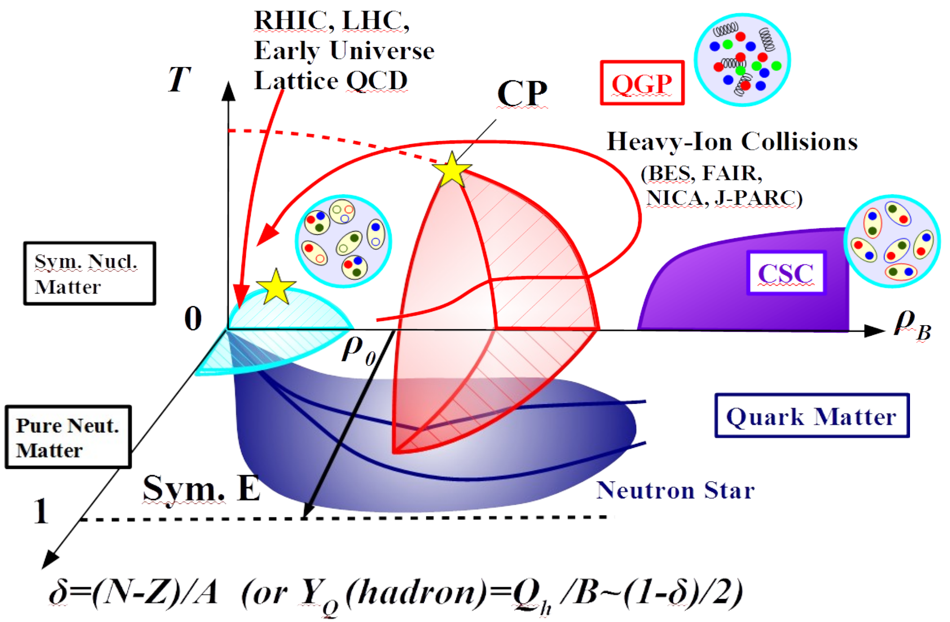
**Kouji Kashiwa (Fukuoka Inst. Tech.)**

*Y. Mori, K. Kashiwa, AO, PRD 96 ('17), 111501(R) [arXiv:1705.05605]*
*Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [arXiv:1709.03208]*
*AO, Y. Mori, K. Kashiwa, EPJ Web Conf. 175 ('18), 07043 [arXiv:1712.01088, Lattice 2017 proceedings]*
*Y. Mori, K. Kashiwa, AO, PLB, in press [arXiv:1705.03646]*
*K. Kashiwa, Y. Mori, AO, arXiv:1805.08940.*
*Y. Mori, K. Kashiwa, AO, in prog.*

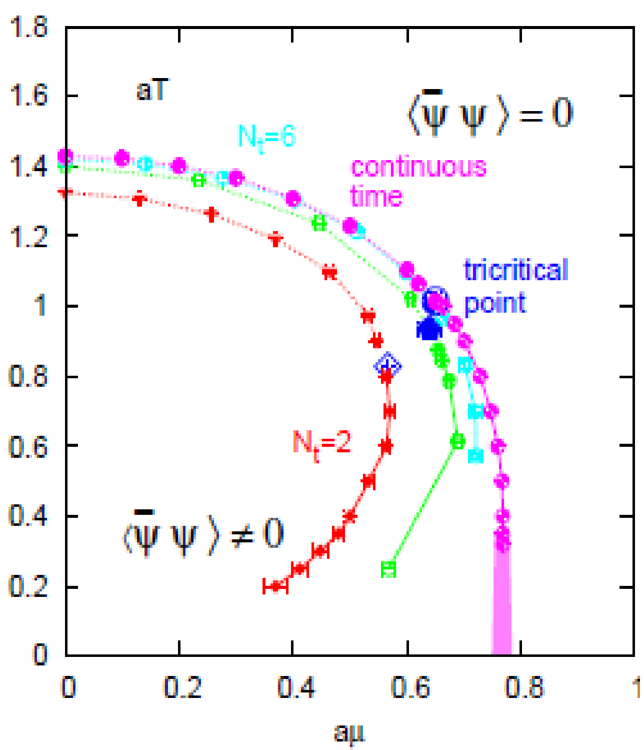
# Introduction

- 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, …

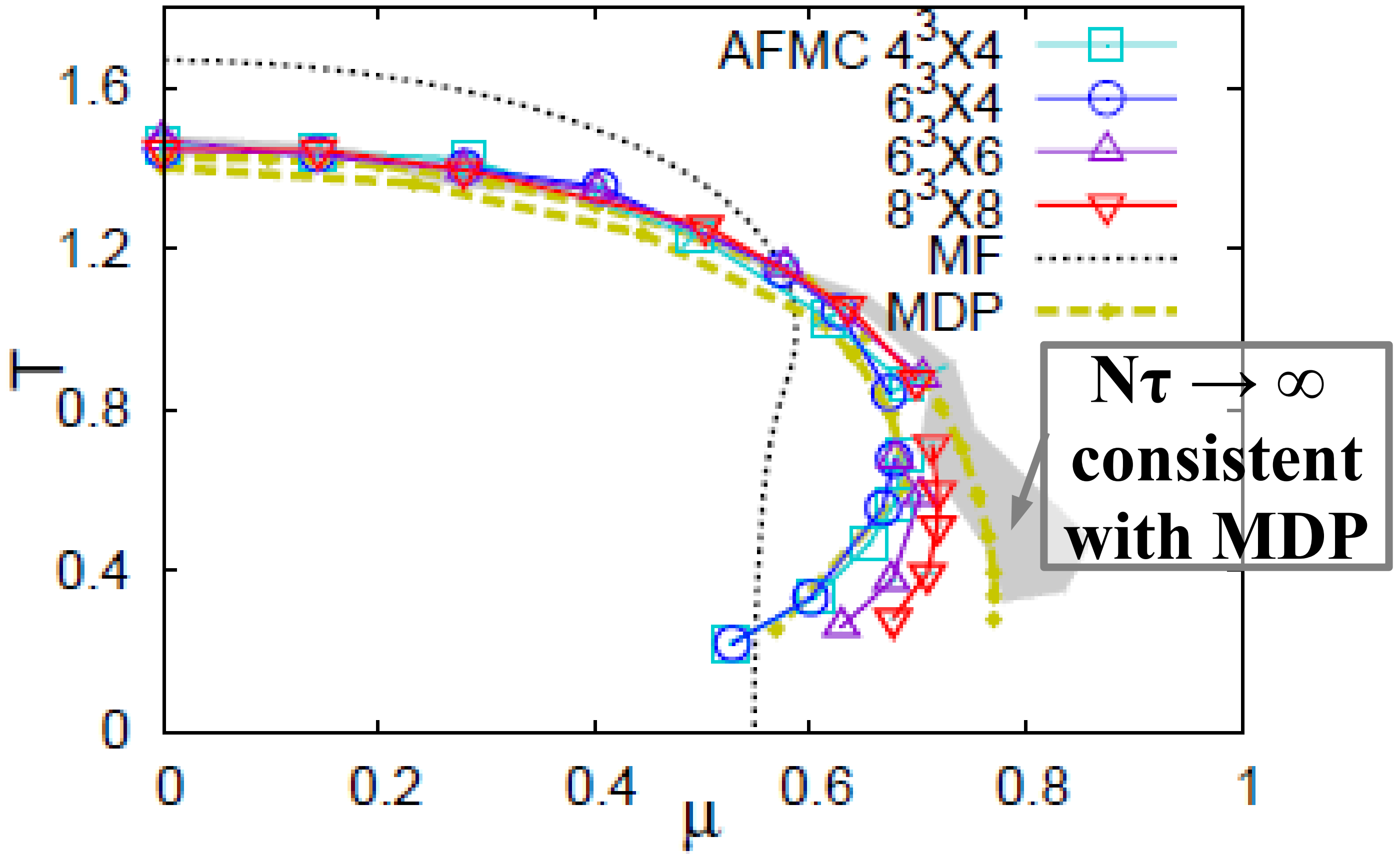


# Phase diagram

- **Phase diagrams in two independent methods (MDP & AFMC) agree with each other in the strong coupling limit.**
  **→ SCL phase diagram is determined !**



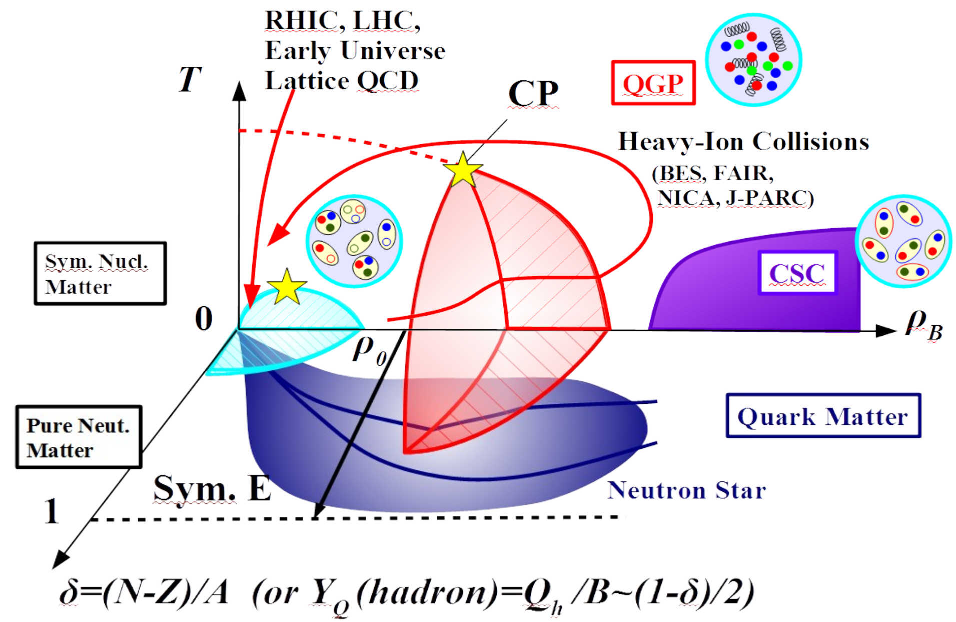

*de Forcrand, Fromm ('10), de Forcrand, Langelage, Philipsen, Unger ('14)*




*Ichihara, AO, Nakano ('14)*

# 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)**
  *Parisi ('83), Klauder ('83), Aarts et al. ('11), Nagata et al. ('16)*
- **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*

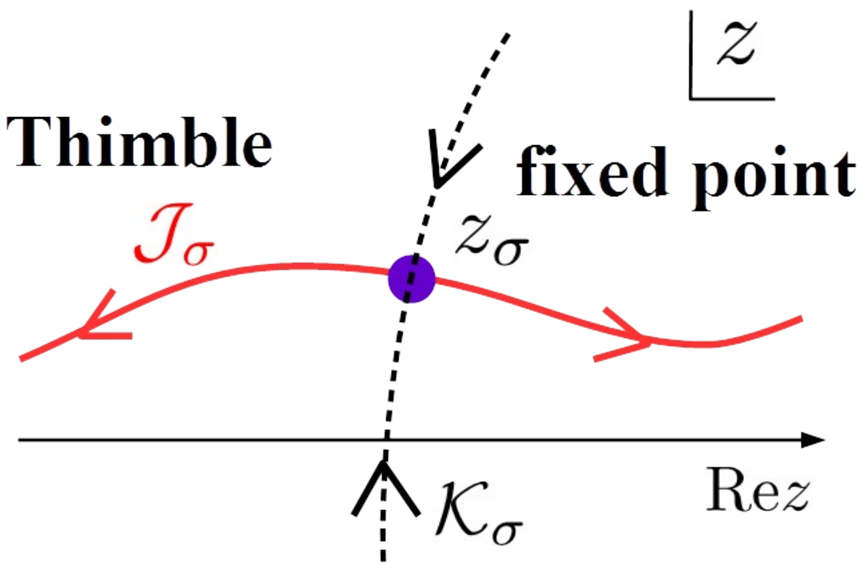
*E. Witten ('10), Cristoforetti et al. ('12), Fujii et al. ('13)*

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

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

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

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

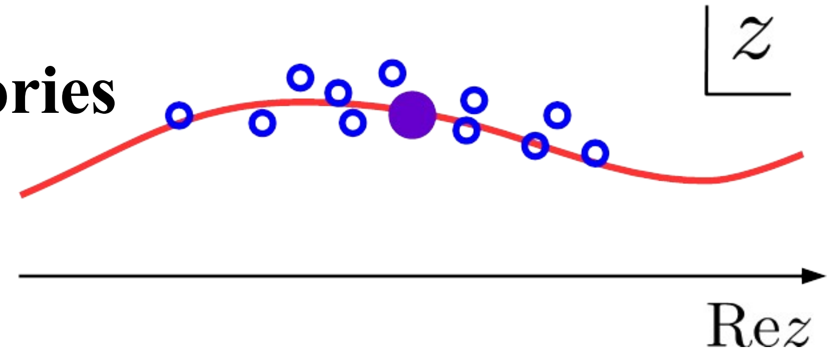



- **Problems**
  - **How can we find fixed points ?** *Alexandru et al., JHEP 1605 ('16) 053*
  - **Phase from measure (residual sign prb.)**
  - **Cancellation between thimbles (global sign prb.)**
  - **Flow equation blows up somewhere.**

# Complex Langevin Method

*Parisi ('83), Klauder ('83), Aarts et al. ('11), Nagata et al. ('16)*

- **Sample configurations by solving complex Langevin equation for complexified variables.**
  **→ Easier to apply to large DOF theories**




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

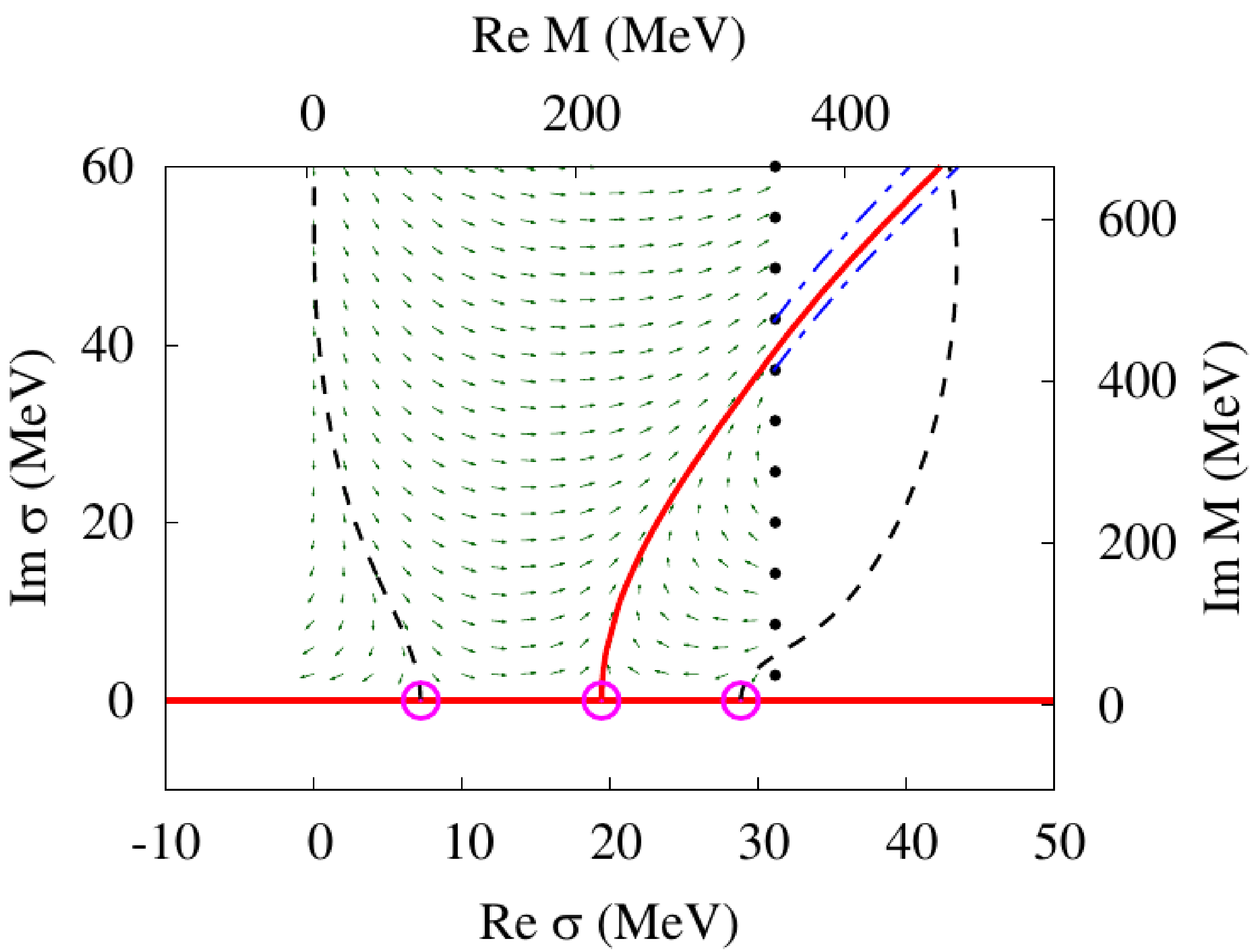
$$\langle \eta_i(t)\eta_j(t)\rangle = 2\delta_{ij}\delta(t-t')$$

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

- **Problems**
  - **Excursion problem → Gauge Cooling** *(Seiler et al. ('13))*
  - **Converged results can be wrong**
    **→ Criteria** *(Nagata, Nishimura, Shimasaki ('16))*
  - **Singular drift problem → Deformation** *(Ito, Nishimura ('16))*

# *Can we avoid singular points of the action ?*

- **There are many singular points of the action in the complexified variable space, especially around the phase transition boundary.**




*Y. Mori, K. Kashiwa, AO, PLB, in press [arXiv:1705.03646]*

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

***Our proposal: Path Optimization***

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  *(Lattice 2017 proceedings)*
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# *Path Optimization Method*

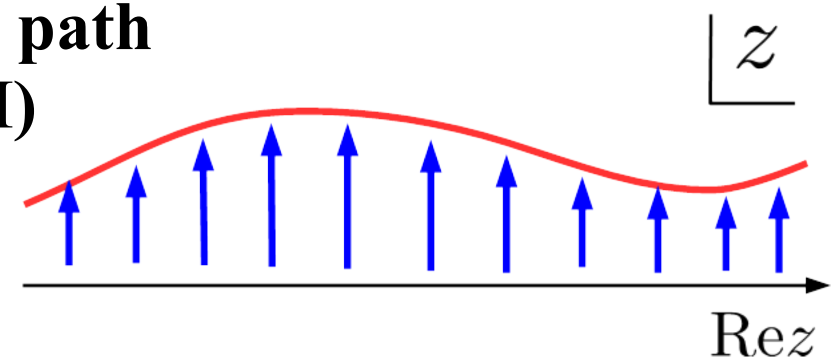
*Y. Mori, K. Kashiwa, AO, PRD 96 ('17), 111501(R) [arXiv:1705.05605]*

*AO, Y. Mori, K. Kashiwa, EPJ Web Conf. 175 ('18)07043*

*[arXiv:1712.01088, Lattice 2017 proceedings]*

# *Path Optimization Method*

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



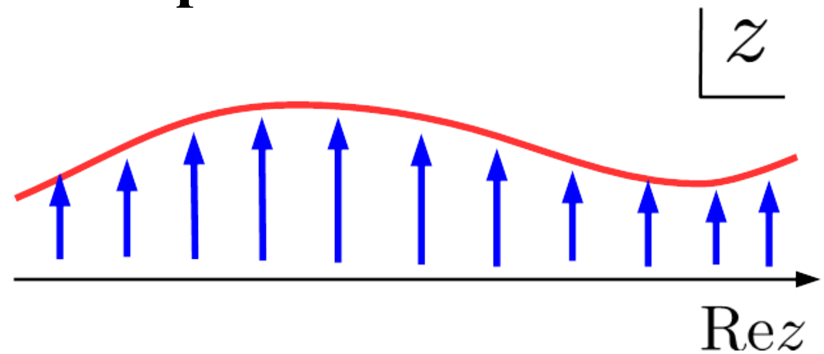

- **POM Procedure**
  - **Parametrize the path appropriately (Trial Function)**
  - **Set a measure of sign problem (Cost Function)**
  - **Tune parameters to minimize the Cost Function (Optimization)**

***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**

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




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

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

$$F[z(t)] = \frac{1}{2} \int dt \left| e^{i\theta(t)} - e^{i\theta_0} \right|^2 \left| J(t) e^{-S[z(t)]} \right|$$

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

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

# *Benchmark test: 1D integral*

*Y. Mori, K. Kashiwa, AO, PRD 96 ('17), 111501(R) [arXiv:1705.05605]*

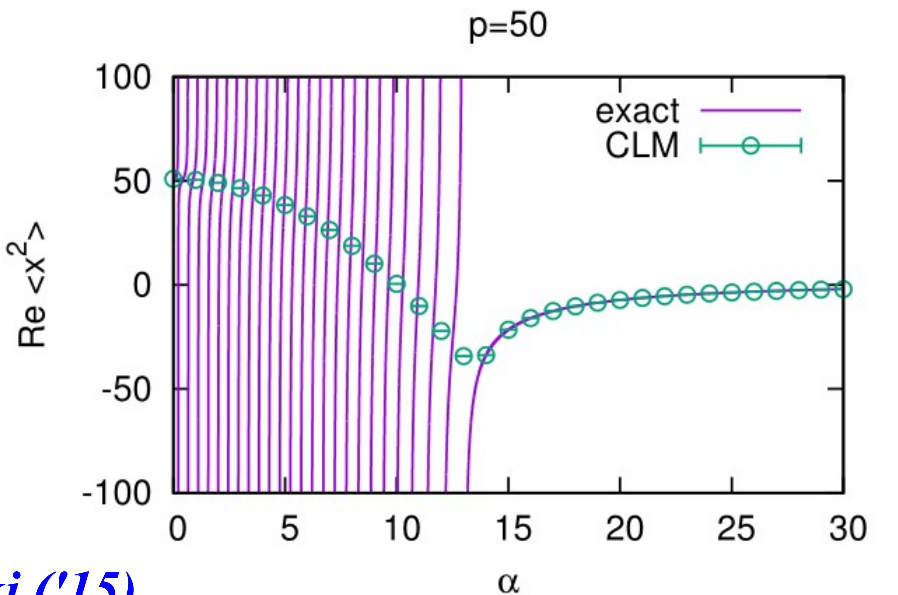
# *A (Pathological) Toy Model*

- **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**




*J. Nishimura, S. Shimasaki ('15)*

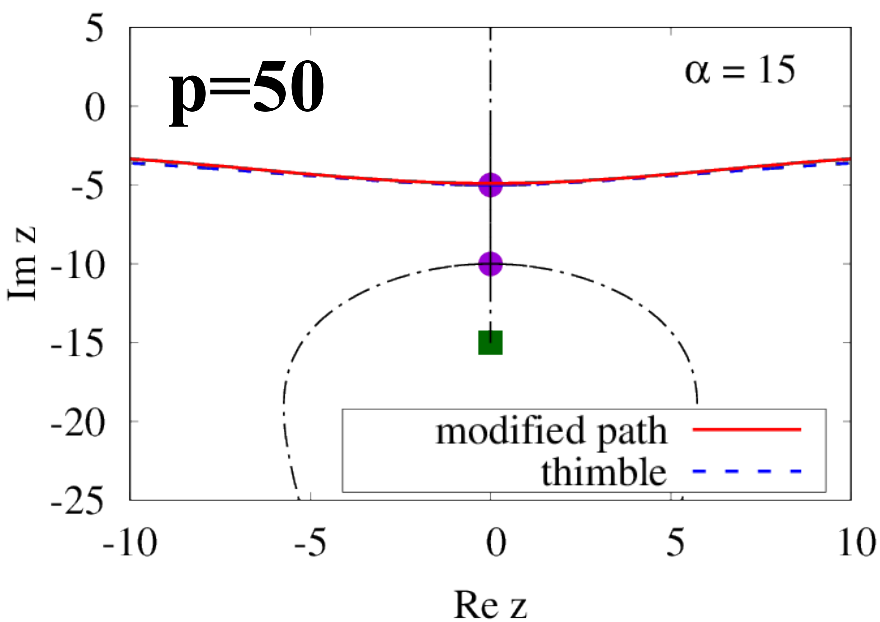
# *Optimized Path*

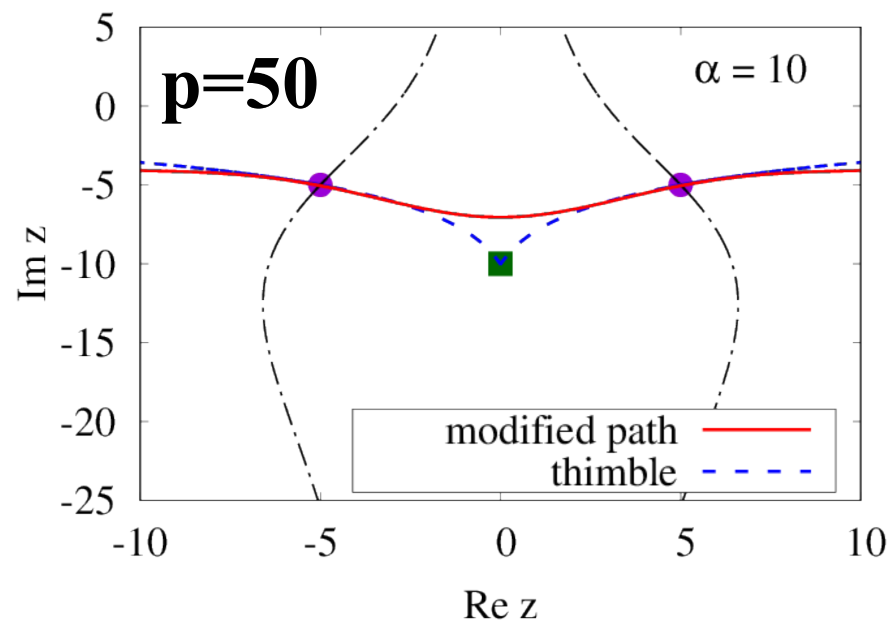
- **Trial Function**

*Mori, Kashiwa, AO ('17)*

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

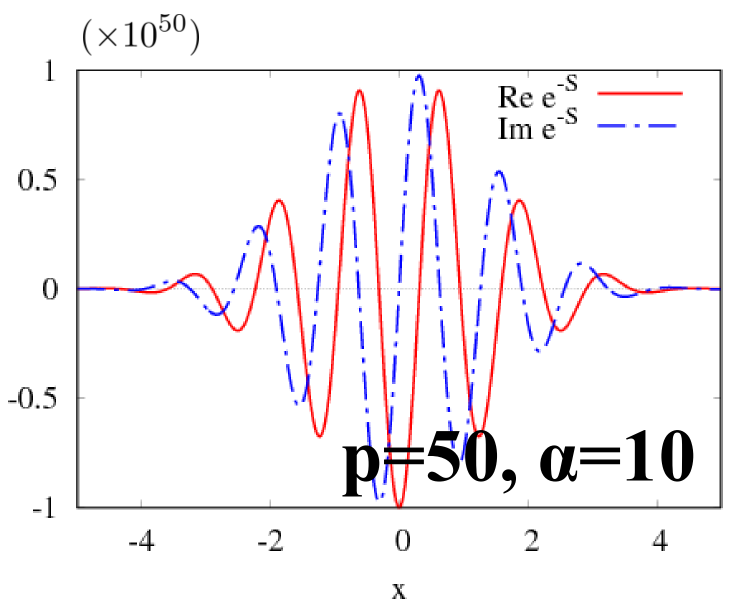
- **Optimization = Gradient descent**
- **Optimized path agrees with thimble(s) around the fixed point(s) !**
  - **Large α → One thimble, Singular point is far away from thimble**
  - **Small α → Go through two FPs.**



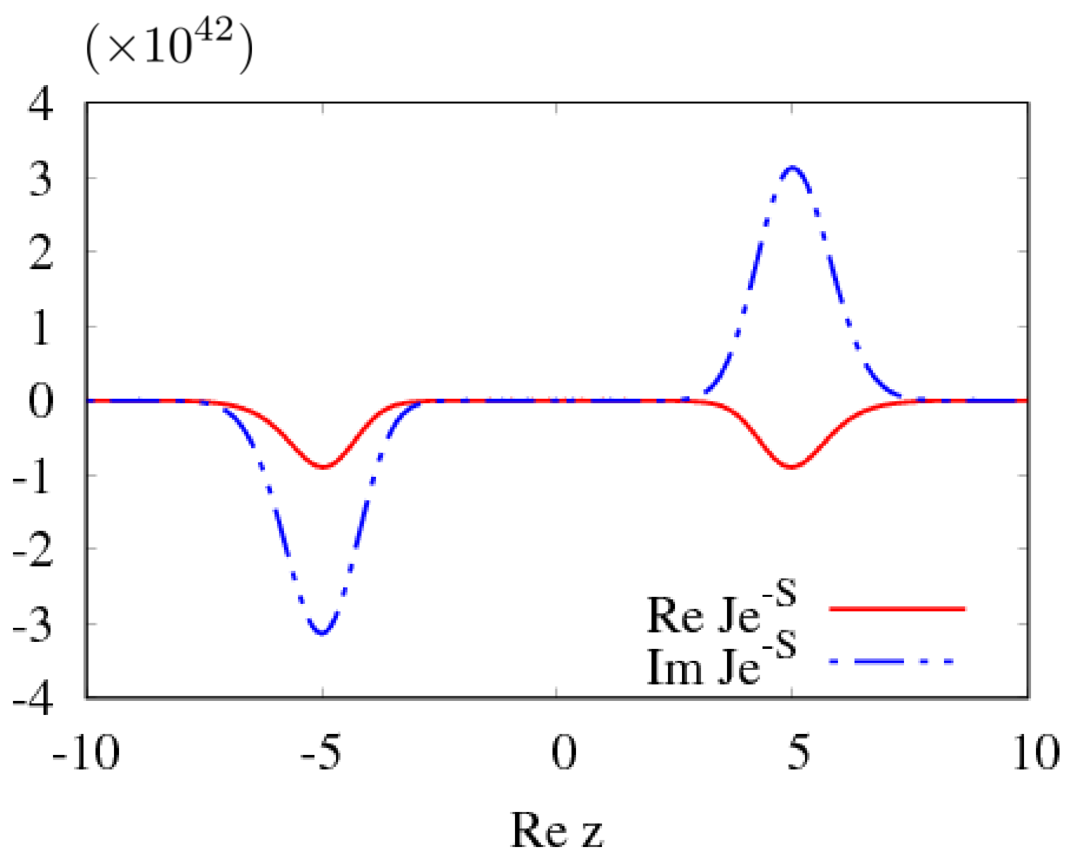



# *Boltzmann Weight*

- **Boltzmann weight ($Je^{-S}$) on the real axis**
  **→ Large (~ $10^{50}$) and rapid oscillation.**
- **$Je^{-S}$ on the optimized path**
  **→ Small (~ a few $10^{42}$) and slow oscillation.**

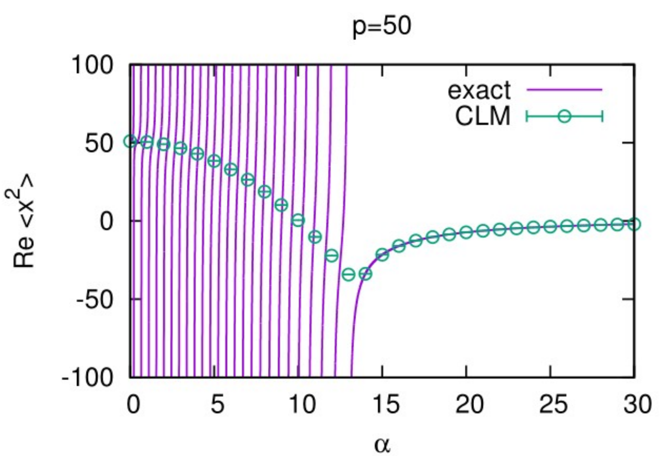



Optimization

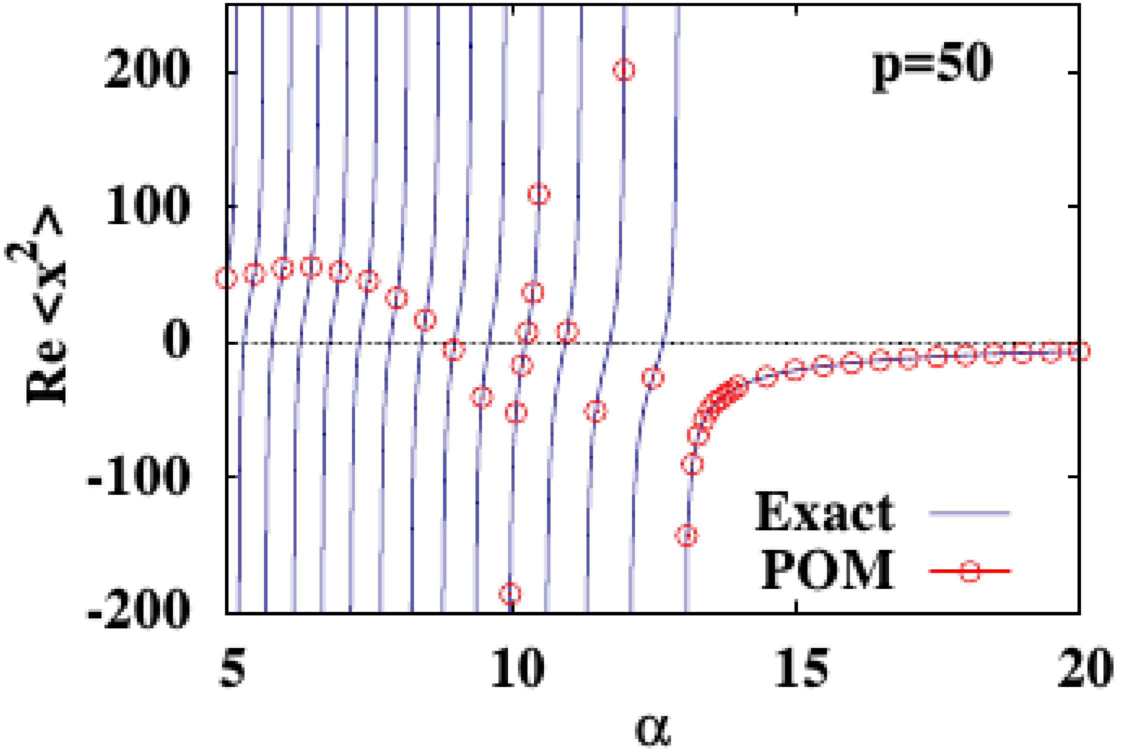


# *Expectation Value of $x^2$*

- **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)*

## *Application to complex $\lambda\varphi^4$ theory with use of neural network*

*Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [arXiv:1709.03208]*

# Application of POM to Field Theory

- **Preparation & variation of trial fn. is tedious in multi-D systems**

$$z_i(t) = t_i + \sum_{n_1,n_2,\dots} (c^{(x)}_{i,n_1 n_2 \dots} + i c^{(y)}_{i,n_1 n_2 \dots}) H_{n_1}(t_1) H_{n_2}(t_2) H_{n_3}(t_3) \cdots$$

- **Neural network**
  - **Combination of linear and non-linear transformation.**

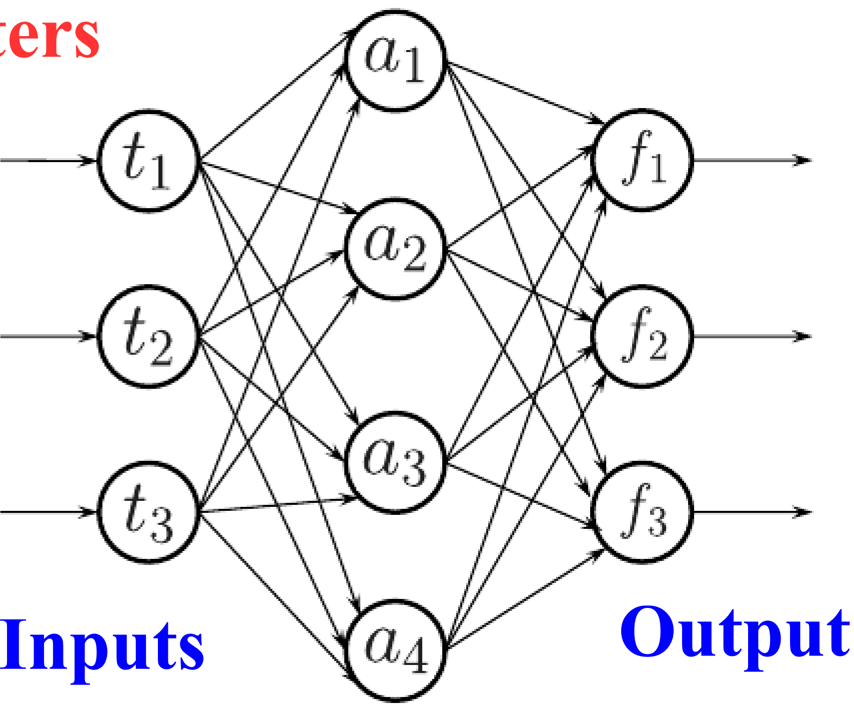
$$a_i = g(\underline{W^{(1)}_{ij}} t_j + \underline{b^{(1)}_i})$$

**parameters**

$$f_i = g(\underline{W^{(2)}_{ij}} a_j + \underline{b^{(2)}_i})$$

$$z_i = t_i + i(\underline{\alpha_i} f_i(t) + \underline{\beta_i})$$

$$g(x) = \tanh x \ (\text{activation fn.})$$




  - **Universal approximation theorem**
    **Any fn. can be reproduced**
    **at (hidden layer unit #) → ∞**
    *G. Cybenko, MCSS 2 ('89) 303*
    *K. Hornik, Neural networks 4('91) 251*

# *Optimization of many parameters*

- **Stochastic Gradient Descent method**
  **E.g. ADADELTA algorithm**
  ***M. D. Zeiler, arXiv:1212.5701***

**par. in (j+1)th step**

**Learning rate**

$$c_i^{(j+1)} = c_i^{(j)} - \eta v_i^{(j+1)}$$

**mean sq. ave. of v**

$$v_i^{(j+1)} = \frac{\sqrt{s_i^{(j)} + \epsilon}}{\sqrt{r_i^{(j+1)} + \epsilon}} F_i^{(j)}$$

**decay rate**

**mean sq. ave. of F**

$$r_i^{(j+1)} = \gamma r_i^{(j)} + (1-\gamma)(F_i^{(j)})^2$$

$$s_i^{(j+1)} = \gamma s_i^{(j)} + (1-\gamma)(v_i^{(j+1)})^2$$

**gradient evaluated in MC (batch training)**

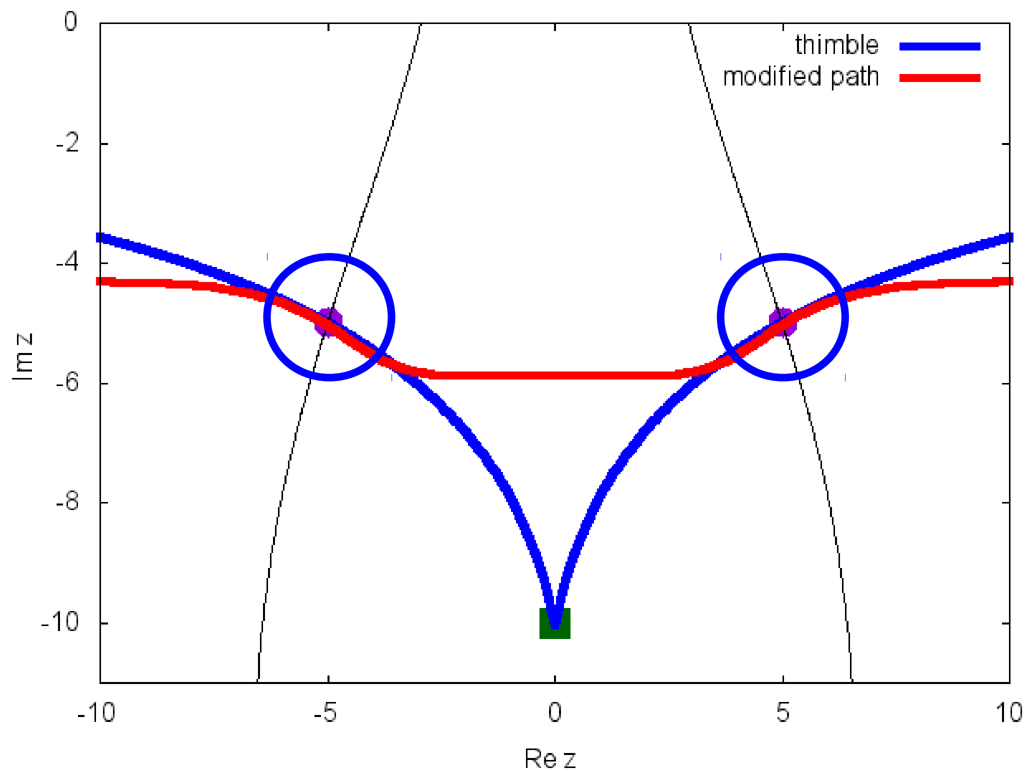
$$F_i = \partial \mathcal{F} / \partial c_i$$

**Cost fn.**

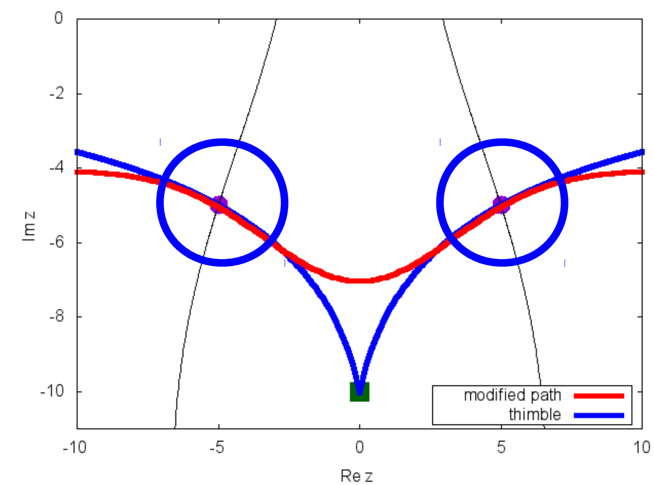
***Machine learning***
***~ Educated algorithm to generic problems***

# *Optimized Path by Neural Network*

**Neural Network**




**Gaussian +Gradient Descent**




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

*AO, Mori, Kashiwa (Lat 2017)*

# *Complex $\lambda\varphi^4$ theory at finite $\mu$*

- **Complex $\lambda\varphi^4$ theory**

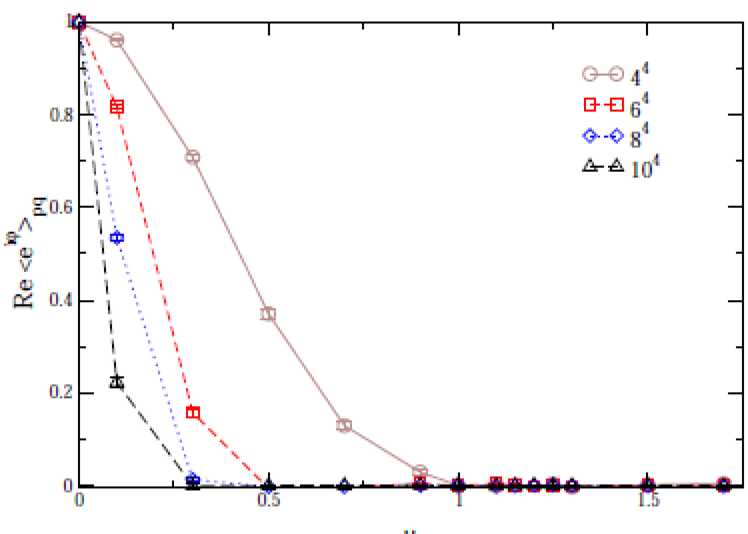
$$\mathcal{L} = \partial_\mu \phi^* \partial^\mu \phi - m^2 \phi^* \phi - \lambda (\phi^* \phi)^2$$

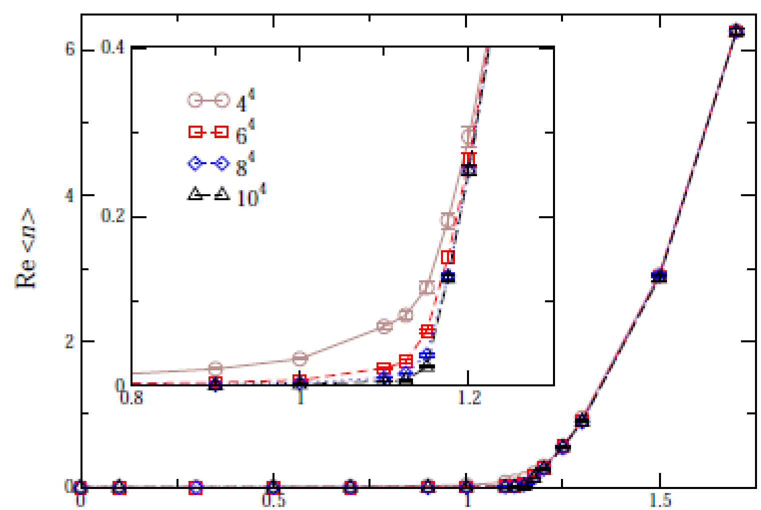
- **Action on Eucledean lattice at finite μ.**

$$S = \sum_x \left[ \frac{(4+m^2)}{2} \phi_{a,x}\phi_{a,x} + \frac{\lambda}{4}(\phi_{a,x}\phi_{a,x})^2 - \phi_{a,x}\phi_{a,x+\hat{1}} \right.$$

$$\left. - \phi_{a,x}\phi_{b,x+\hat{0}}(\delta_{ab}\cosh(\mu) - \underline{i\epsilon_{ab}\sinh(\mu)}) \right] \quad \left( \phi = \frac{1}{\sqrt{2}}(\underline{\phi_1} + i\underline{\phi_2}) \right)$$

**complex** **Complexify**



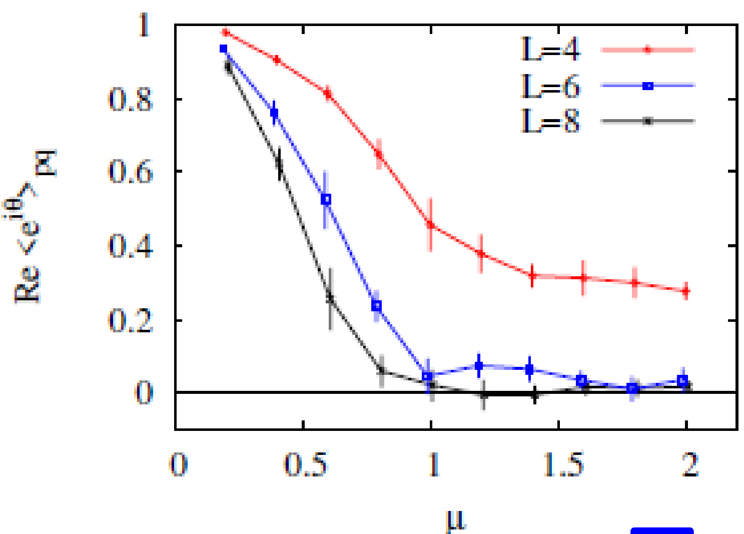




**Complex Langevin & Lefschetz thimble works.**

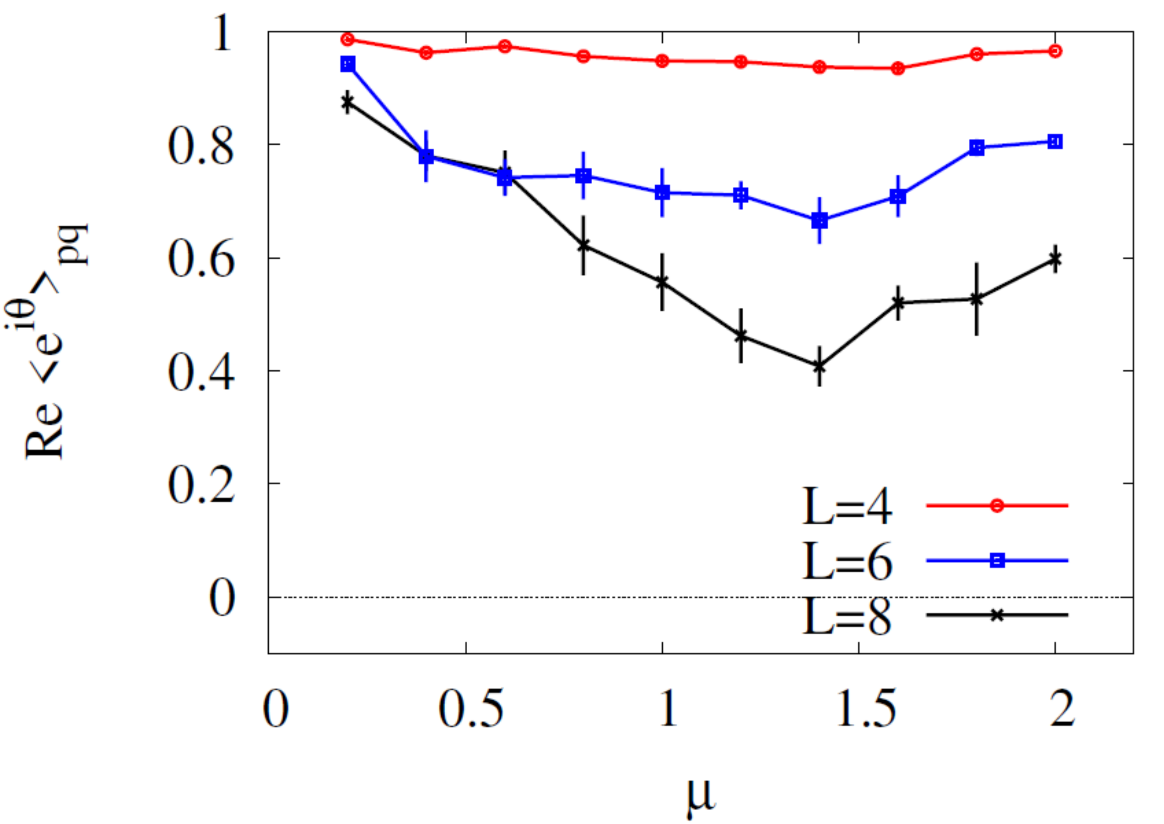
*G. Aarts, PRL102('09)131601; H. Fujii, et al., JHEP 1310 (2013) 147*

# *POM result (1): Average phase factor*

- **POM for 1+1D $\lambda\varphi^4$ theory**
  - **$4^2$, $6^2$, $8^2$ lattices, $\lambda$=m=1**
  - **$\mu_c \sim 0.96$ in the mean field approximation**
  - **Enhancement of the average phase factor after optimization.**








*Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [arXiv:1709.03208]*

# POM result (2): Density

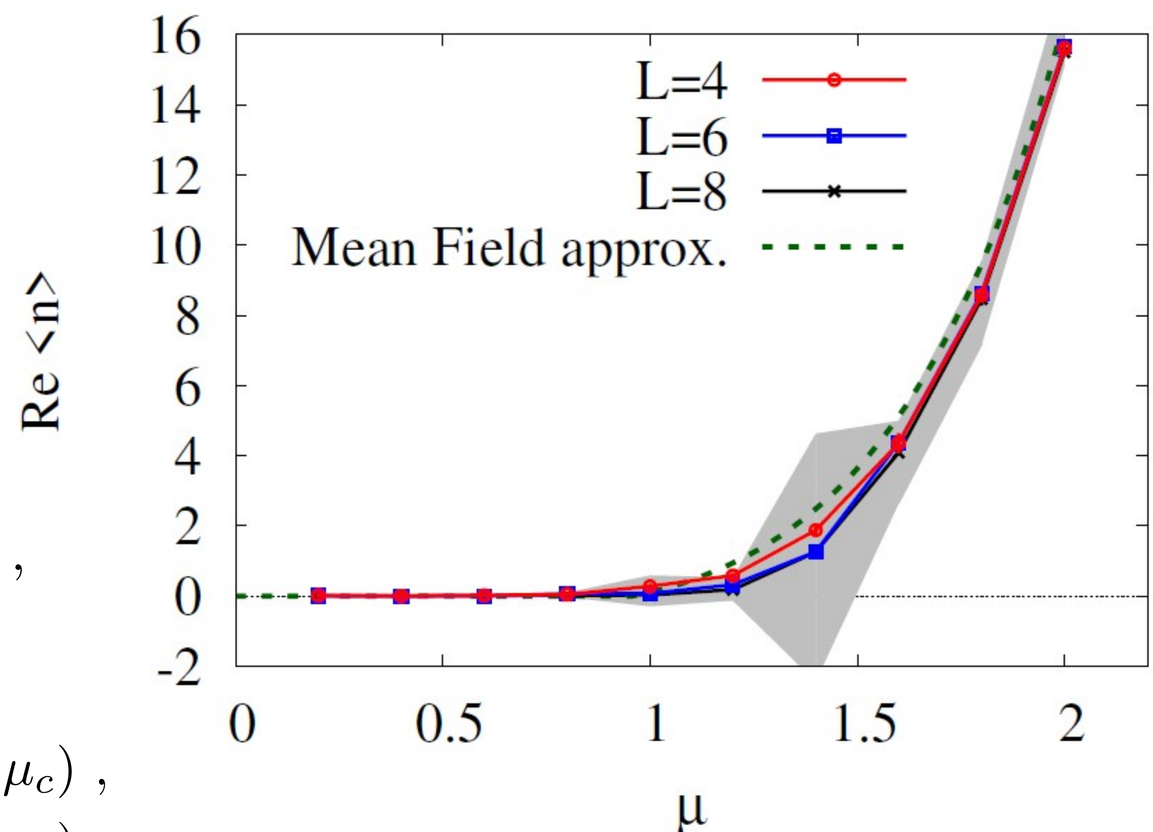
- **Results on the real axis**
  **Small average phase factor, Large errors of density**
- **On the optimized path**
  **Finite average phase factor, Small errors**

**Mean Field App.**

$$\frac{S}{V} = \left(1 + \frac{m^2}{2} - \cosh\mu\right)\phi^2 + \frac{\lambda}{4}\phi^4 \ ,$$

$$n = \phi^2 \sinh\mu \ ,$$

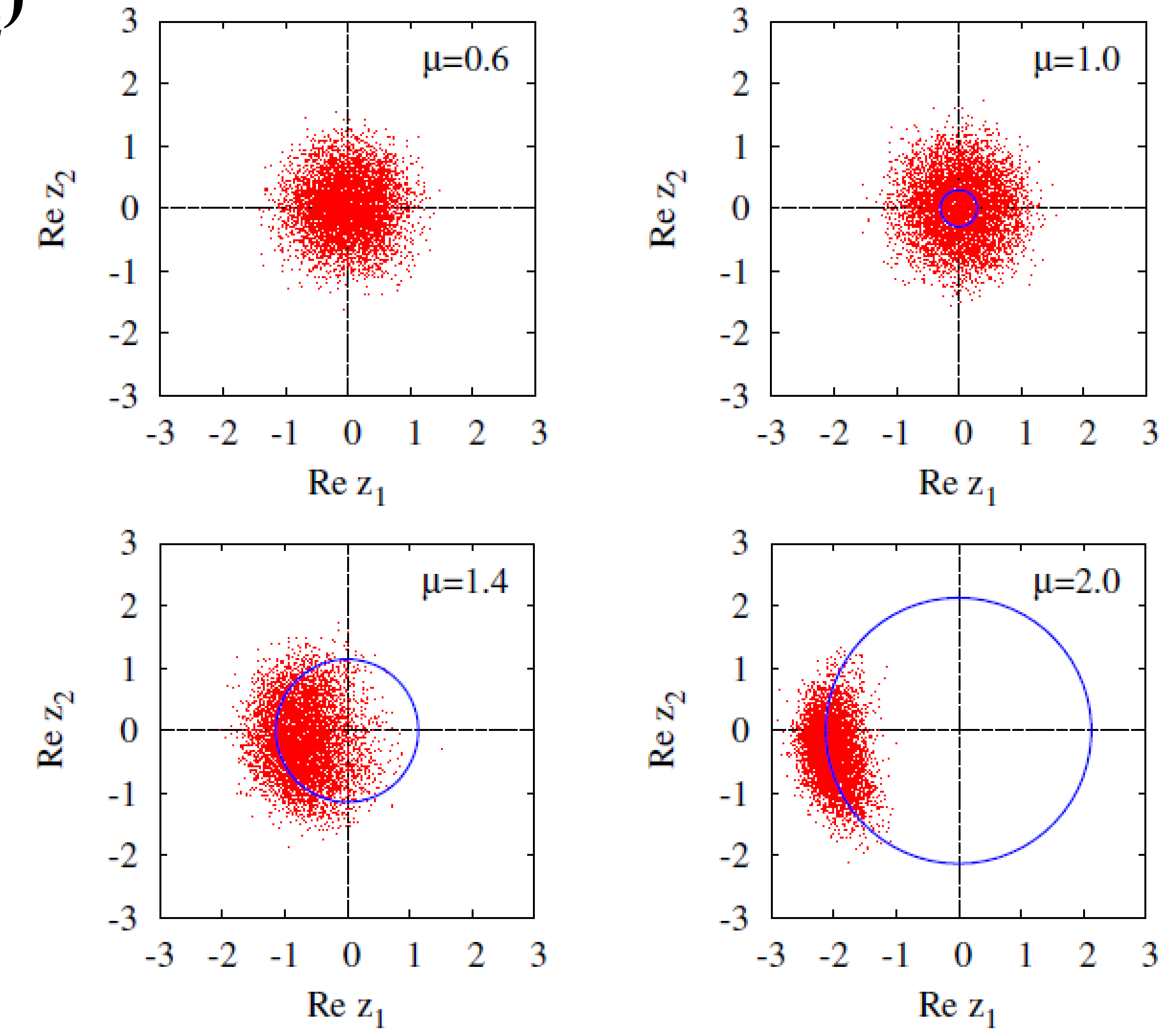
$$\phi^2_{\mathrm{stat.}} = \begin{cases} 0 & (|\mu| < \mu_c) \ , \\ \frac{2}{\lambda}\left(\cosh\mu - 1 - \frac{m^2}{2}\right) & (|\mu| \geq \mu_c) \ , \end{cases}$$




*Mori, Kashiwa, AO ('18)*

# *POM result (3): Configurations*

- **Updated configurations after optimization**
  **→ sampled around the mean field results**
- **U(1) symmetry in ($\varphi_1$, $\varphi_2$) is broken spontaneously by the optimization ? (or by the sampling)**



# *Prospects of path optimization*

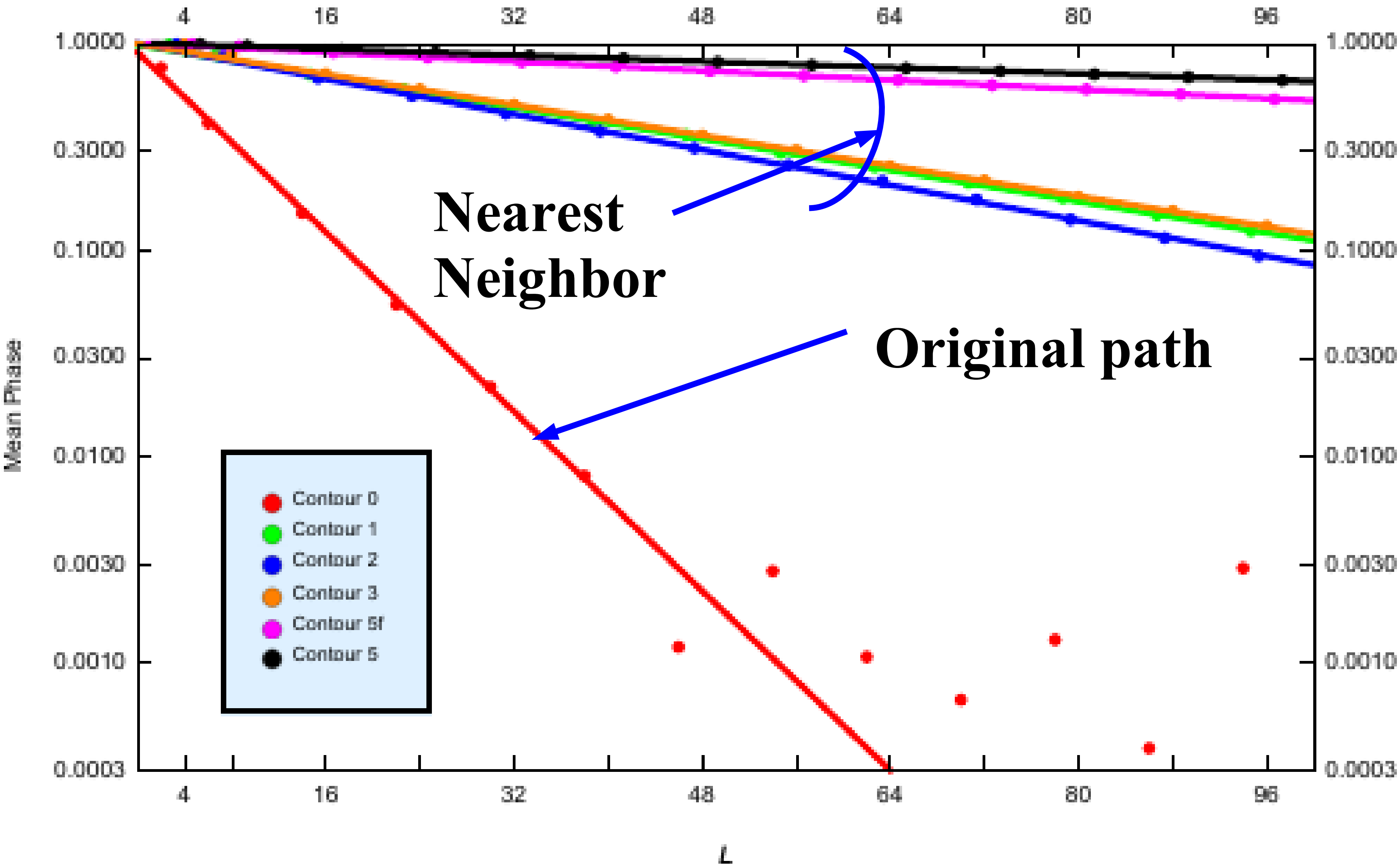
# *Problems in Path Optimization*

- **Merits**
  - **Optimization of the path including Jacobian**
  - **Singular points of the "Action" do not matter in many cases(*).**
    **(* Singularity coming from zeros of Fermion determinant does not harm path optimization.)**
- **Problem**
  - **Optimization is not trivial even with neural network.**
  - **Large number of parameters to be optimized, $O((N_{dof})^2)$.**
  - **Huge CPU times would be necessary, $O((N_{dof})^3)$ for Jacobians.**
    **→ Reduced pars. assuming nearest neighbor correlation**
    *F. Bursa, M. Kroyter, arXiv:1805.04941*

    **→ Jacobian only from the same site ? (We doubt it !)**
    *A. Alexandru et al., PRD96 ('17), 094505 [arXiv:1709.01971];*
    *A. Alexandru et al., PRD97('18), 094510 [arXiv:1804.00697].*

# *Optimization with Nearest Neighbor Site Correlation*

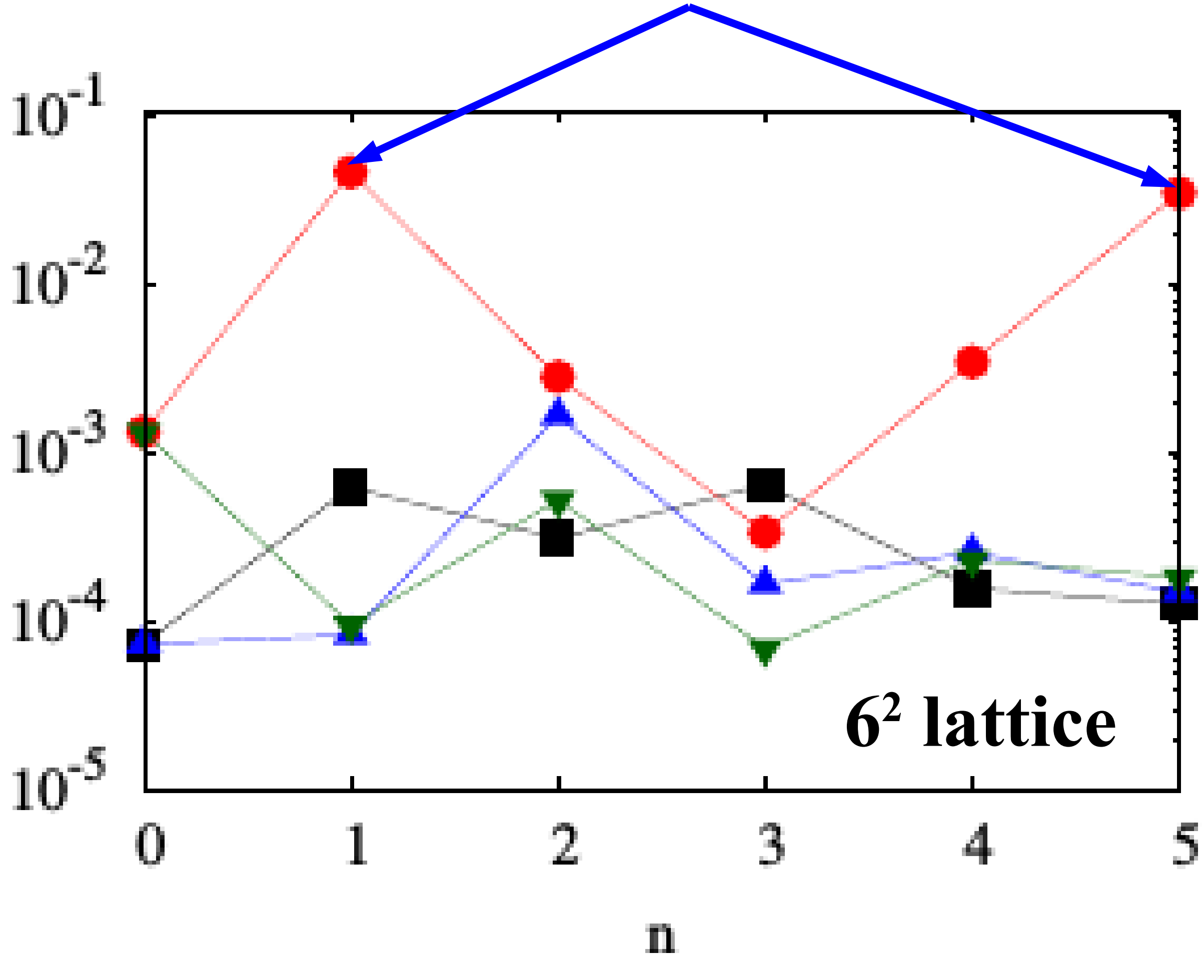
- **Economical optimization with sparse Jacobian matrix.**
  *F. Bursa, M. Kroyter, arXiv:1805.04941*



# *Nearest Neighbor Site Correlation Dominates ?*

- **Yes, in complex $\lambda\varphi^4$. Other correlations $\sim 10^{-1}$-$10^{-2}$ times smaller**
- **Hope to reduce the cost to be $O(N_{dof})$**

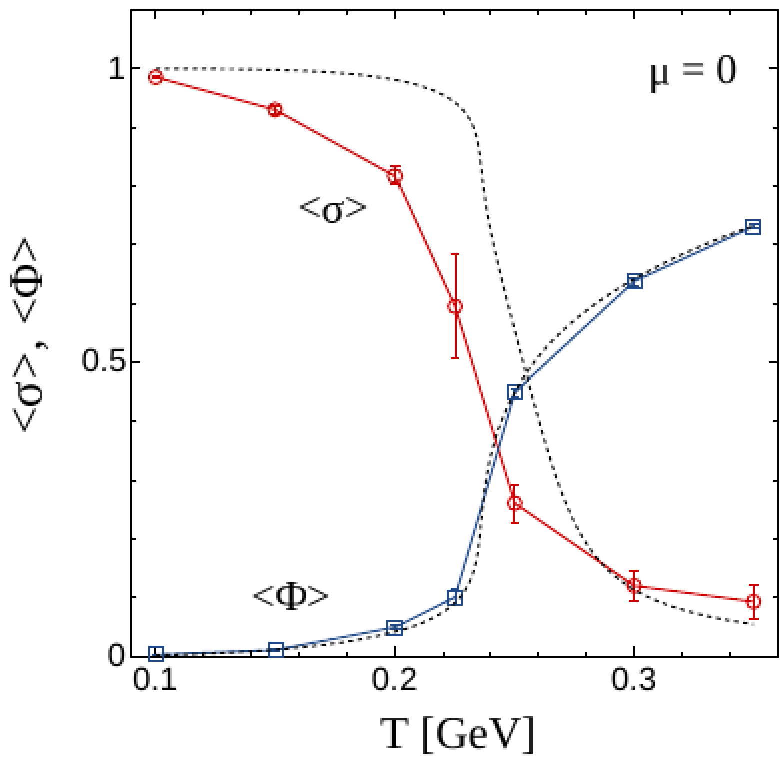
**($\varphi_1$, $\varphi_2$) nearest temporal neighbor site corr.**

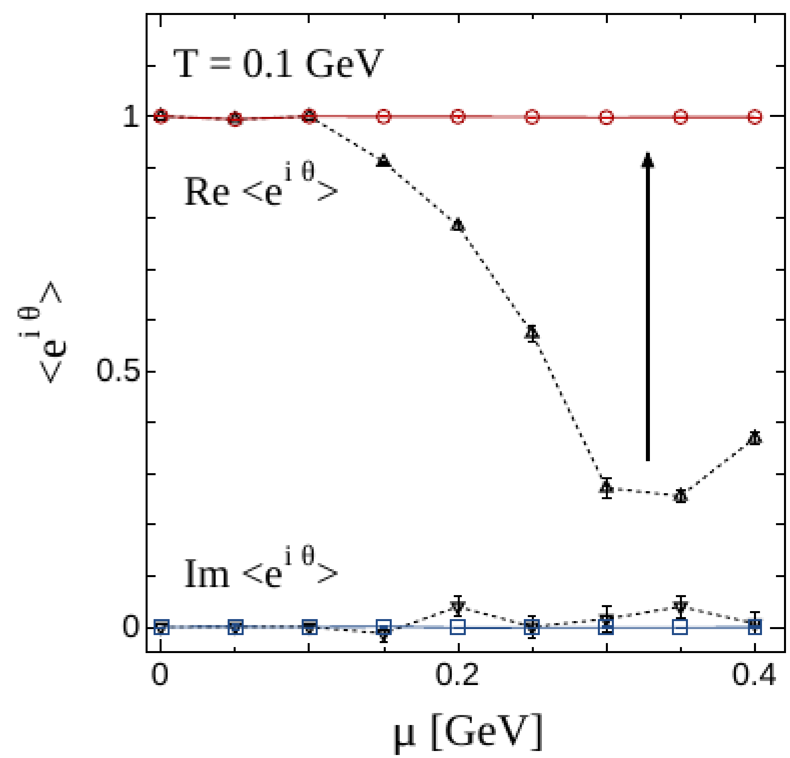



*Y. Mori, Master thesis*

# Application to PNJL

- **PNJL model with homogeneous condensates, ($\sigma$, $\pi$, $\Phi$, $\bar{\Phi}$).**
  - **Has Sign problem in finite volume**
  - **Converges to mean field results in the large volume limit**




*K. Kashiwa, Y. Mori, AO, arXiv:1805.08940.*

# *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 several models.**
  - **Optimized path reproduces the thimble(s) around the fixed point(s).**
  - **Many of singular points of the action do not matter, as long as they are not the singular points of the Boltzmann weight.**
  - **Global sign problem is unsolved (and should not be solved).**
- **POM is applicable to field theories with use of neural network.**
- **Simplification based on sparse Jacobian matrix seems to be promising.**

# *Application to Gauge Theories*

- **2D SU(2) Yang-Mills theory with complex coupling**
  *K. Nagata, J. Nishimura and S. Shimasaki, arXiv:1802.01876 [hep-lat],*
  *H. Makino, H. Suzuki and D. Takeda, PRD92 ('15)085020.*
  **→ Struggling ….**