Two topics in the sign problem – Lefschetz thimbles in NJL and the path optimization method –

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in collaboration with
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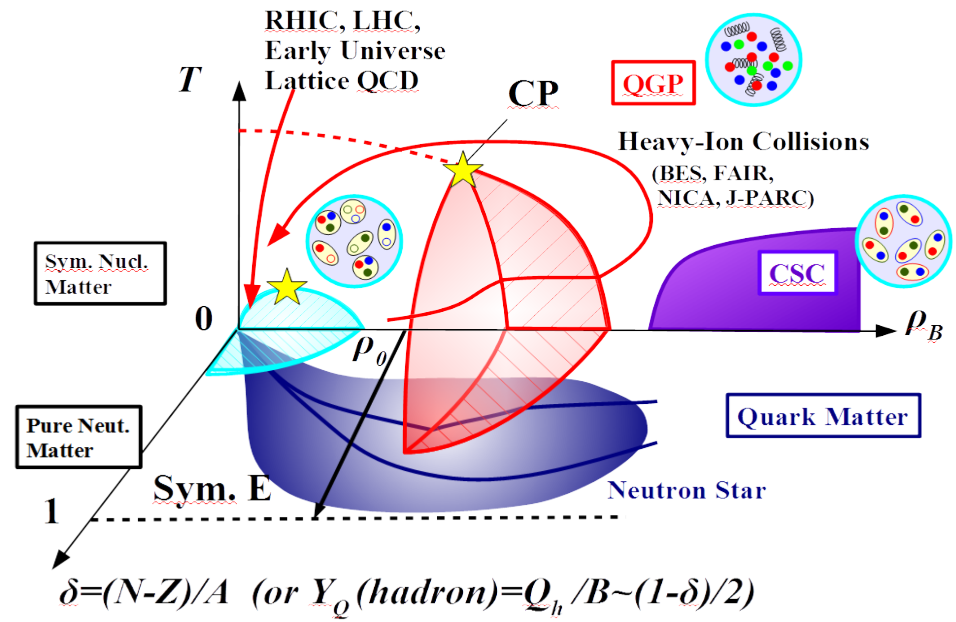
KEK Theory Center Seminar, July 18, 2017

(1) Lefschetz thimbles in fermionic effective models with repulsive vector-field
Yuto Mori, Kouji Kashiwa, Akira Ohnishi, arXiv:1705.03646 [hep-lat].
(2) Toward solving the sign problem with path optimization method
Yuto Mori, Kouji Kashiwa, Akira Ohnishi, arXiv:1705.05605 [hep-lat].

Introduction

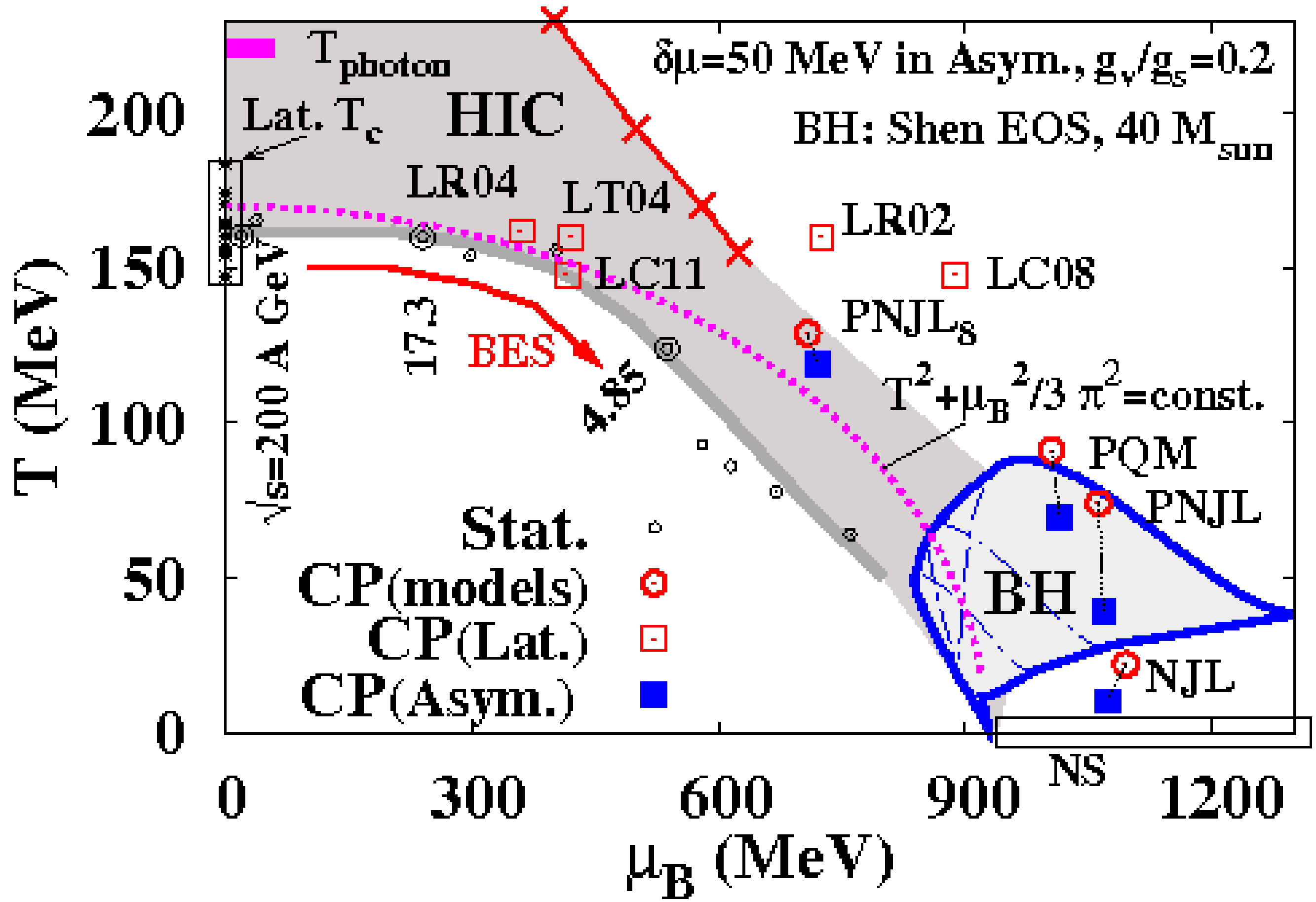
- **Sign problem for complex actions**
  - **Grand challenge in theor. phys.**
  - **Largest obstacle to explore QCD phase diagram**



Physics of Dense QCD

- Finite nuclei from QCD (Dream of nuclear physicists)
- Nuclear matter EOS, Nuclear symmetry energy, Strangeness Nuclear Phys., …
  → Neutron star matter EOS
- Hadrons in medium
  → (Partial) restoration of chiral sym. and $U(1)_A$ sym.
- QCD phase transition at finite ρ (critical point, 1st order p.t.)
  → Phase diagram, Massive neutron star puzzle, …
- Charm hadron physics, Charm nuclear physics

QCD phase diagram (Exp. & Theor. Studies)

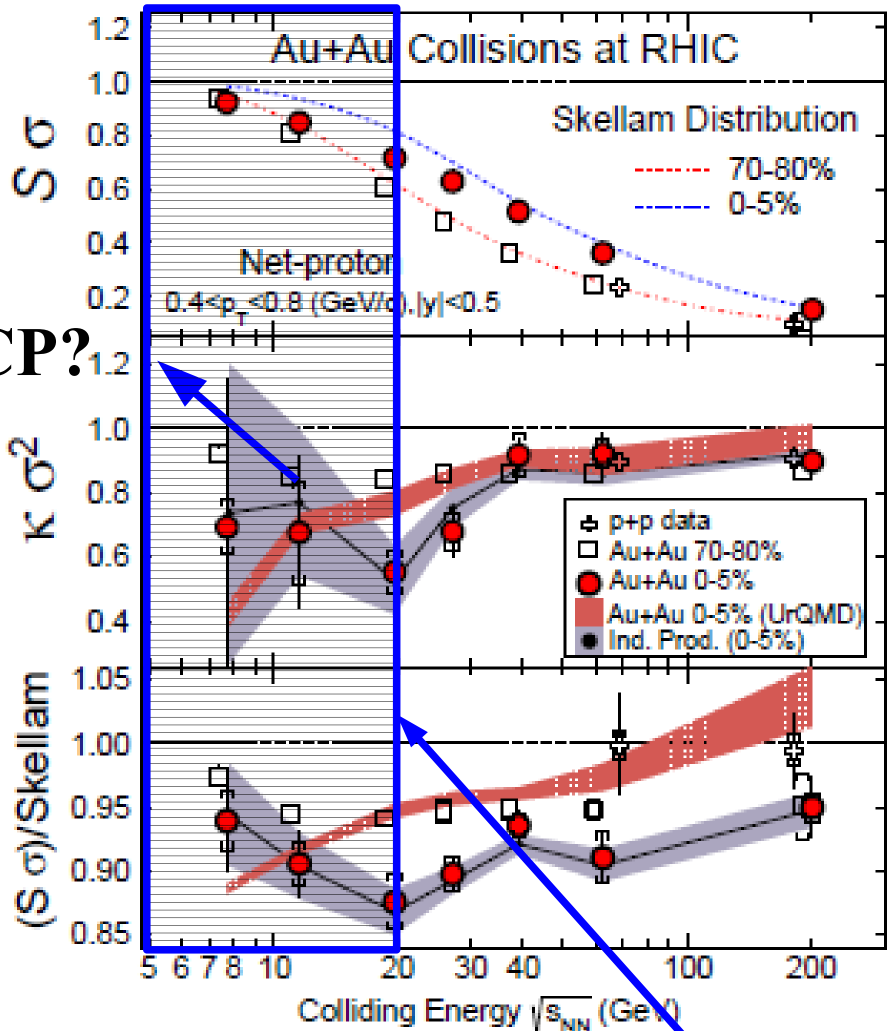


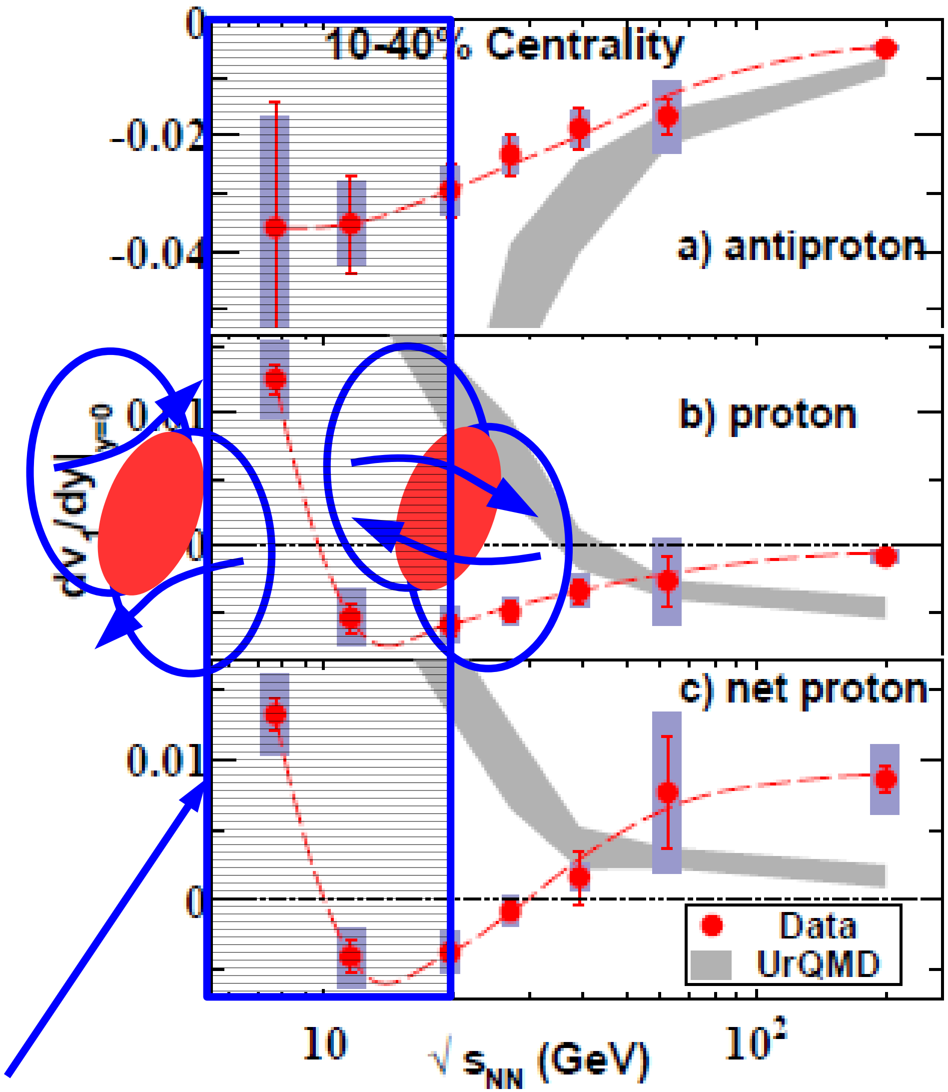
QCD phase transition is not only an academic problem, but also a subject which would be measured in HIC or Compact Stars

AO, PTPS 193('12)1

Net-Proton Number Cumulants & Directed Flow

CP?





"J-PARC" energies

Non-Poisson Dist.

STAR Collab. PRL 112('14)032302

Softeing of EOS

STAR Collab., PRL 112('14)162301.

Physics of Dense QCD

- **Finite nuclei from QCD (Dream of nuclear physicists)**
- **Nuclear matter EOS, Nuclear symmetry energy, $\boxed{\text{Strangeness Nuclear Phys.}}$, …**
  → Neutron star matter EOS
- **$\boxed{\text{Hadrons in medium}}$**
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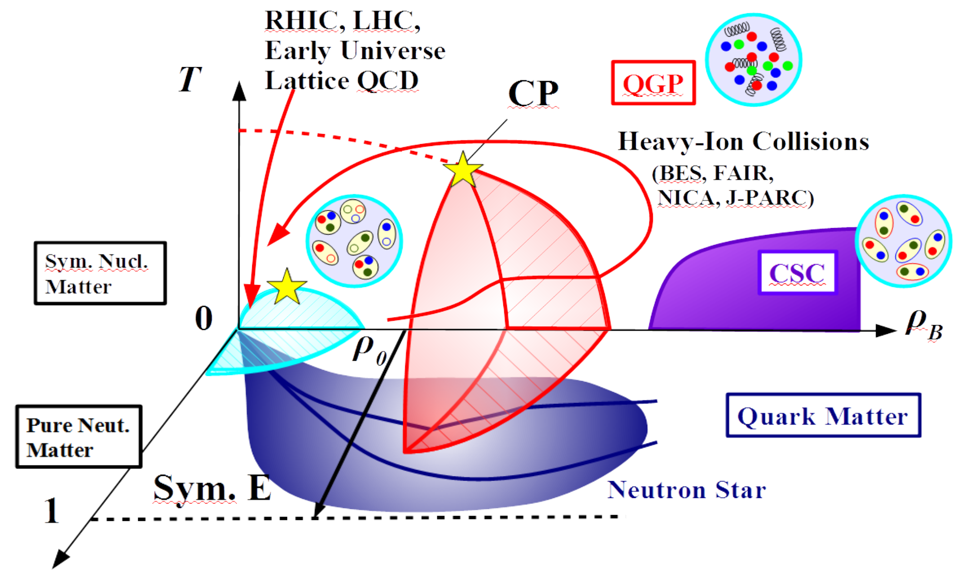
- **$\boxed{\text{QCD phase transition at finite } \rho \text{ (critical point, 1st order p.t.)}}$**
  → Phase diagram, Massive neutron star puzzle, …
- **$\boxed{\text{Charm hadron physics, Charm nuclear physics}}$**

J-PARC (KEK-JAEA) can serve as a dense QCD machine !

Introduction

- Sign problem for complex actions
  - Grand challenge in theor. phys.
  - Largest obstacle to explore QCD phase diagram
- Approaches to finite ρ LQCD
  - 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)

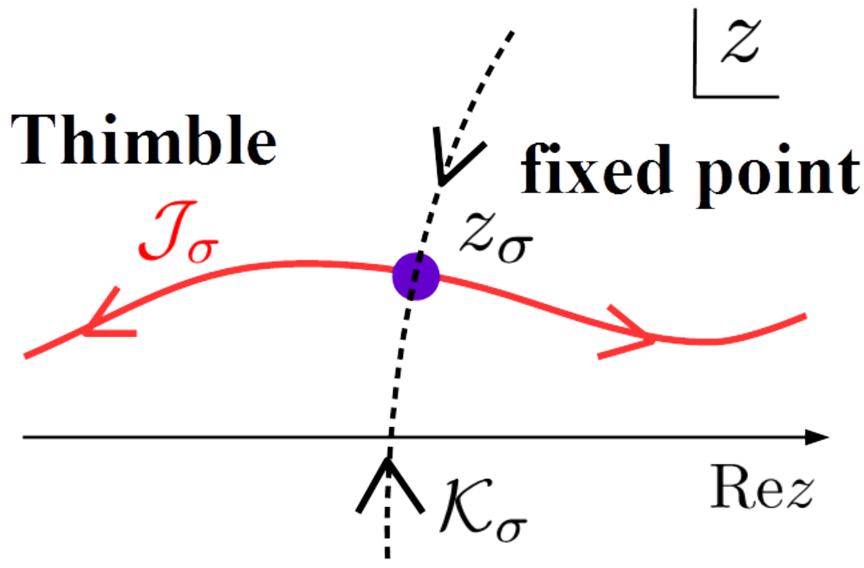
Lefschetz Thimble Method

- **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.**

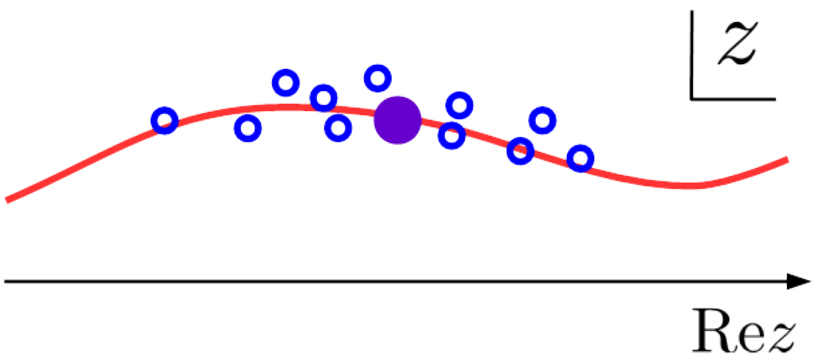
Complex Langevin Method

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

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

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

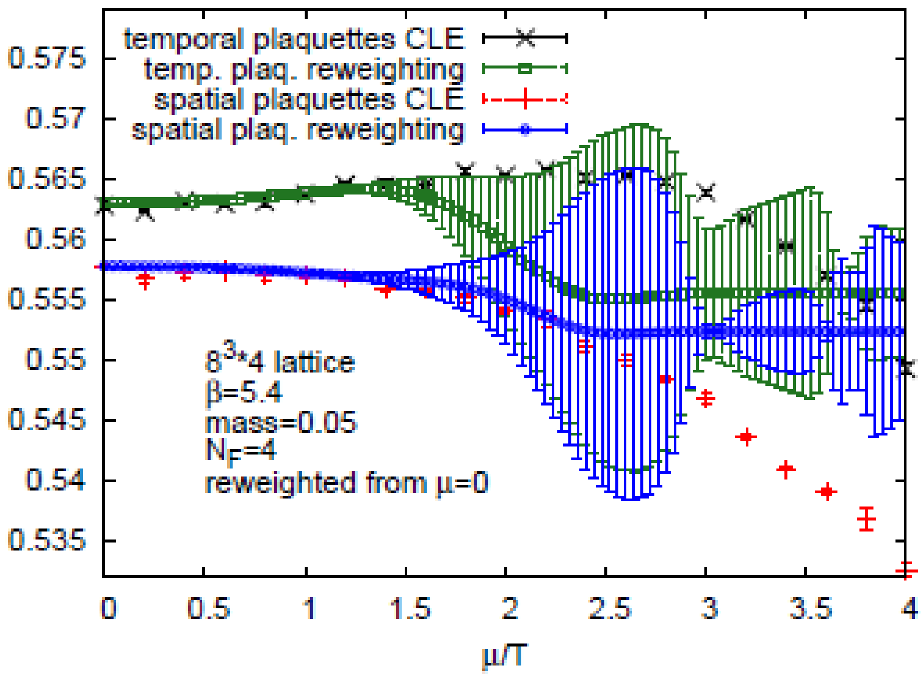
$$\langle \mathcal{O}(x)\rangle = \langle \mathcal{O}(z)\rangle$$

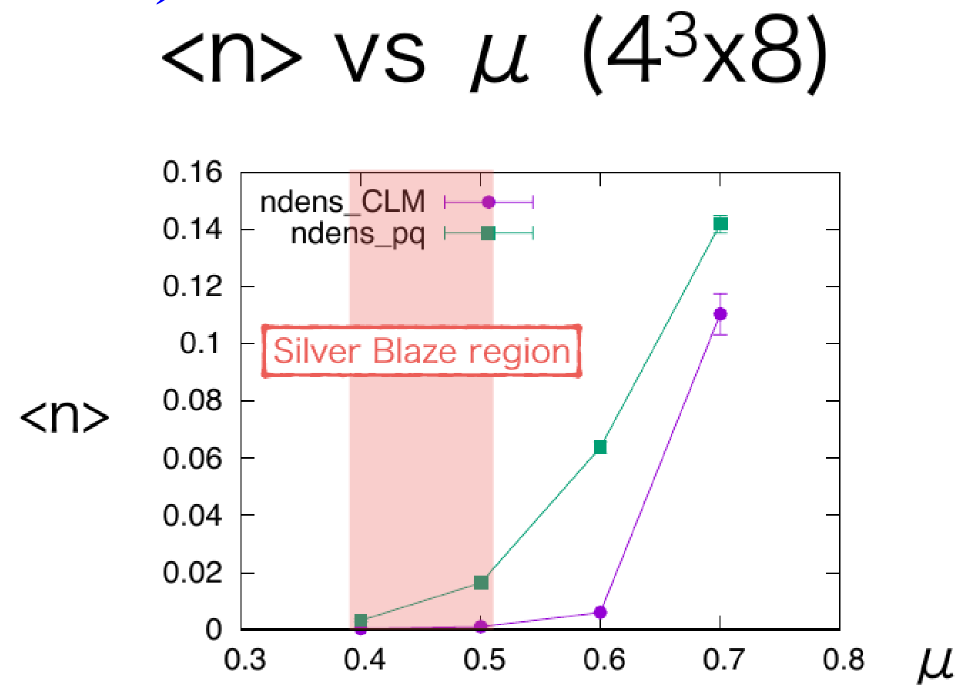


- **Pros**
  - **Easier to apply to large DOF theories**
- **Cons**
  - **Excursion problem → Gauge Cooling** *(Seiler et al. ('13))*
  - **Converged results can be wrong → Criteria** *(Nagata et al. ('16))*
  - **Singular drift problem → Several prescriptions** *(Ito, Nishimura ('16))*

Finite Density Lattice QCD

- **Are we close to the goal ?**
  - **Complex Langevin with gauge cooling seems to work at low densities.**
    Fodor, Katz, Sexty Torok ('15)
  - **CLM + Gauge Cooling + Deformation may overcome the Silver Blaze problem (density should not grow below $\mu < M_N/3$ at low T).**
    Shimasaki, Nagata, Nishimura (Lat2017)





Shimasaki @ Lattice 2017

Application to the QCD phase transition

- **Possible problems in applying LTM/GLTM/CLM to QCD phase transition at high densities.**
  - **Singular points (poles and cuts) may be close to or on the thimbles. Most of the justifications are given under the assumption of no singularities.**
  - **Global sign problem**
    Two fixed points necessarily appears in the 1st order p.t.
    c.f. Combining thimbles to one [S. Tsutsui, T. M. Doi ('16)]
- **Preparation for the Grand Challenge**
  - **Nambu-Jona-Lasinio model in the mean field approximation.**
    “Standard” model of QCD phase transition.
    Can the field-compliexified approaches describe NJL model phase diagram ?
  - **If not, is there any other approaches ?**

Contents

- **Introduction**
- **Lefschetz thimbles in the NJL model with vector coupling**
  Y. Mori, K. Kashiwa, AO, arXiv:1705.03646 [hep-lat].
- **Path Optimization Method and its application to a Toy Model**
  Y. Mori, K. Kashiwa, AO, arXiv:1705.05605 [hep-lat]
- **Summary**

Lefschetz thimbles in the NJL model with vector interaction

Nambu-Jona-Lasinio (NJL) model

- **NJL model Lagrangian with vector coupling (Euclidean)**

$$\mathcal{L} = \bar{q}(-i\gamma_\mu\partial_\mu + m_0 - \mu\gamma_0)q - G\left[(\bar{q}q)^2 + (\bar{q}i\gamma_5\vec{\tau}q)^2\right]$$
$$+ G_v(q^\dagger q)^2 - G_v(\bar{q}\gamma_i q)^2$$

- **Bosonization of repulsive vector field → complex action**

$$\exp[-G_v(q^\dagger q)^2] = \int d\omega_4 \exp[-G_v\omega_4^2 + 2iG_v\omega_4 q^\dagger q]$$

c.f. "standard" mean field treatment

ω_0 is not a dynamical variable, but a constraint.

$$-G_v(q^\dagger q)^2 = G_v\omega_0^2 - 2G_v\omega_0 q^\dagger q$$

Vector coupling in NJL leads to a complex action.
How does the Lefschetz thimble look like ?

Singularities for complex σ

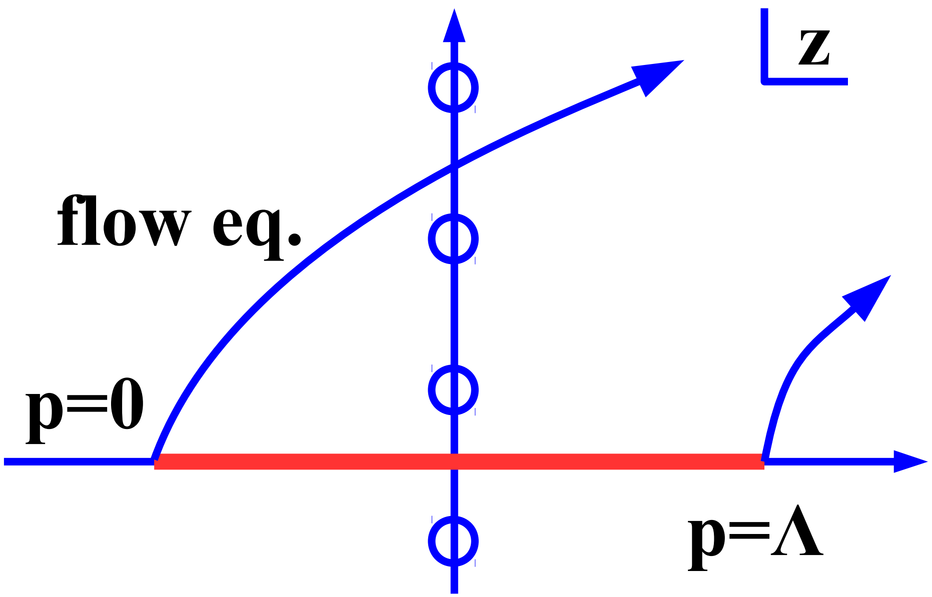
- **Eff. pot. (thermal-particle part, in mean field approx., w/o ω)**

$$\Gamma_{\mathrm{T}} = \frac{N_c N_f}{3\pi^2}\left[\int_0^{\Lambda} \frac{p^4\,dp}{E_p}\frac{1}{1+e^{(E_p-\mu)/T}} - \Lambda^3 T \log(1+e^{-(E_\Lambda-\mu)/T})\right]$$

$$E_p = \sqrt{p^2+M^2}\,, \quad M = m_0 + 2G\sigma$$

- **Singular points with complexified σ**

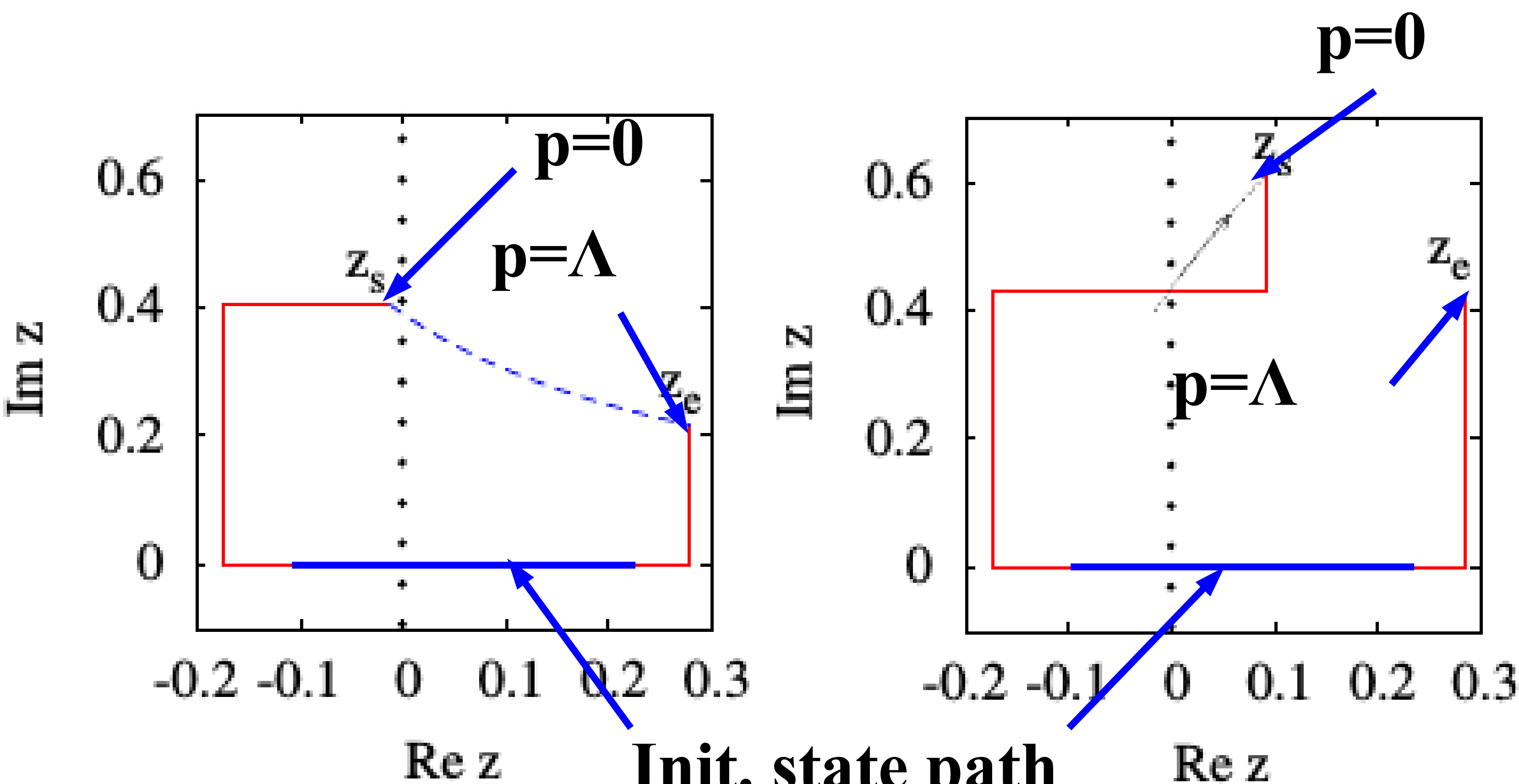
$$z \equiv E_p - \mu = (2k+1)i\pi T$$



How can we determine the momentum integration path ?

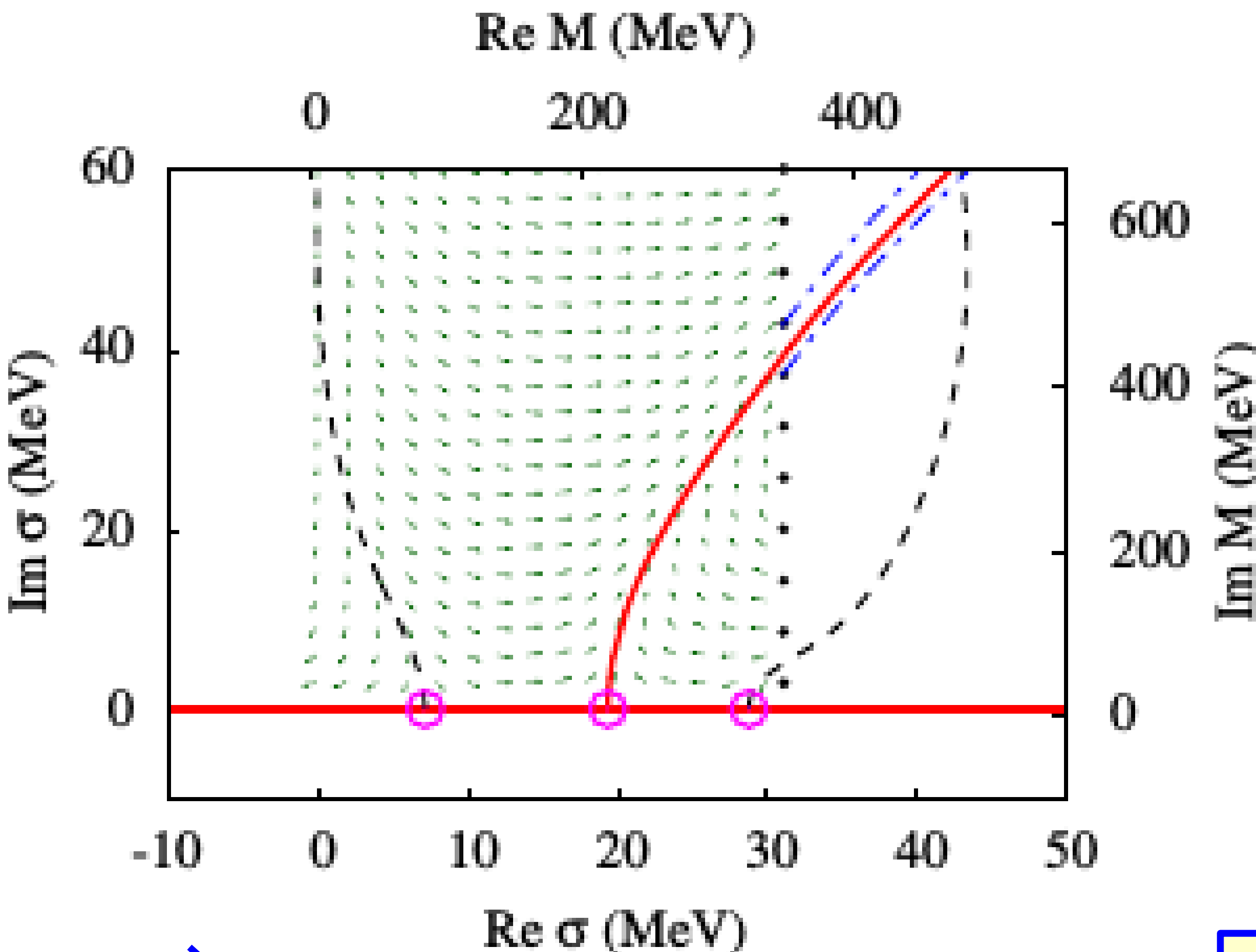
How to define the momentum integration path

- **Grandient flows should run on the same Riemann sheet.**
  - **Integration path should not go across the pole and cuts along the thimble (J and K).**
  - **The "slit" is registered as a function of the fixed point, and the integration path is determined to go through the same slit.**

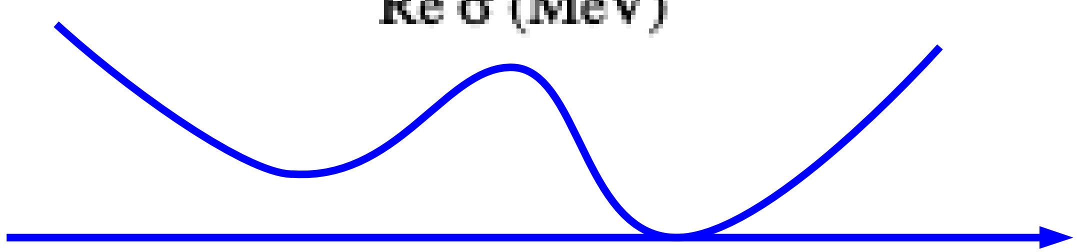


Y. Mori, K. Kashiwa, AO, arXiv:1705.03646.

Lefschetz thimble in NJL



T=10 MeV,
μ=360 MeV
(~ critical μ at T=0)



Relevant thimbles = Real Axis

Y. Mori, K. Kashiwa, AO, arXiv:1705.03646.

Auxiliary Sign Problem

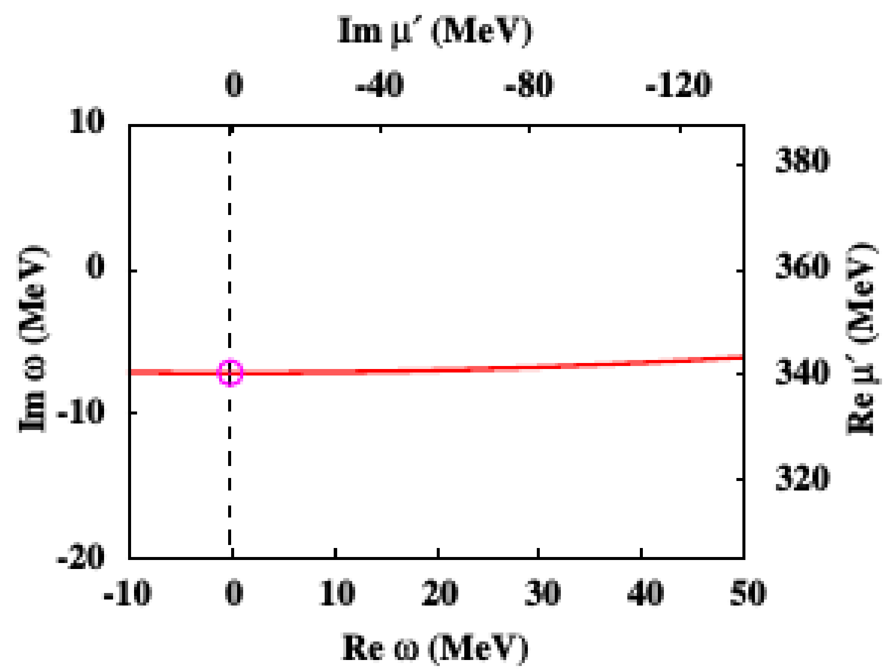
- **Eff. pot. in the mean field approx.**

$$\mathcal{V} = -2N_f N_c \int \frac{d^3p}{(2\pi)^3} \left[E_p + T(\ln f^- + \ln f^+)\right] + G\sigma^2 + G_v\omega_4^2$$

$$f^\mp = 1 + e^{-\beta(E_p \mp \mu')},\ E_p = \sqrt{p^2 + M^2}$$

$$\mathcal{V} = S/V/\beta,\ M = m_0 + 2G\sigma,\ \mu' = \mu - 2iG_v\omega_4$$

- **Fixed point** $\omega_4 = -i\langle q^\dagger q\rangle,\ \mu' = \mu - 2G_v\langle q^\dagger q\rangle$
  - **Eff. pot. is real at fixed points → Justification of MF treatment.**
- **Thimble (with fixed σ)**
  - **Almost parallel to the real axis.**
- **Problem: With both σ and ω are varied, flow eq. stops in a short time. Why ?**



Y. Mori, K. Kashiwa, AO, arXiv:1705.03646.

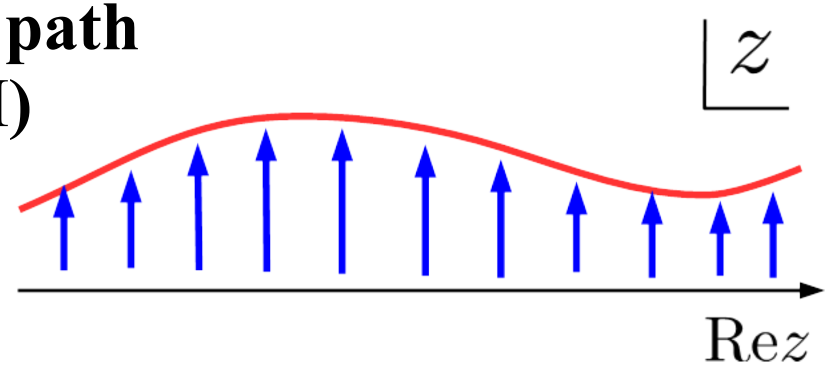
Singular points exist around the fixed points and solving flow equation is not easy in the (bosonized) action of the NJL model, a "standard" model to discuss QCD phase diagram.

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

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)



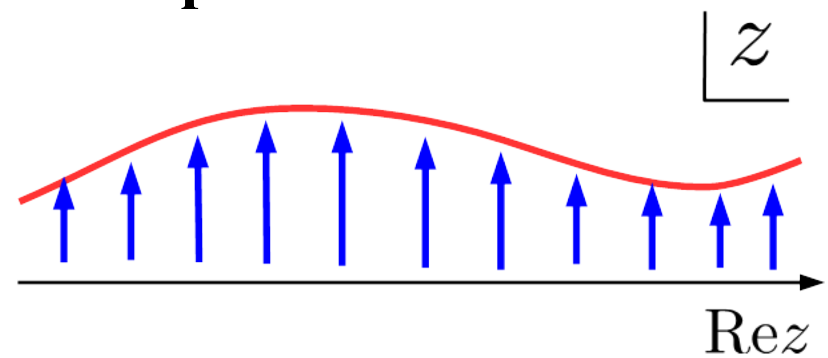
- **POM Procedure**
  - **Parametrize the path appropriately (Trial Function)**
  - **Set a measure of sign problem (Cost Function)**
  - **Tune parameters to minimize the Cost Function (Optimization)**

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**

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



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

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

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

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

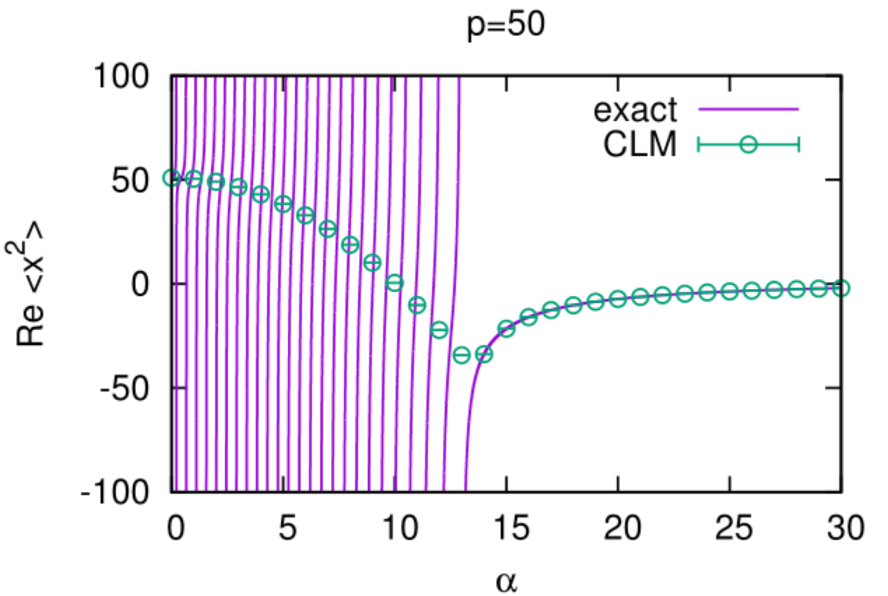
A (Pathological) Toy Model

- **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**



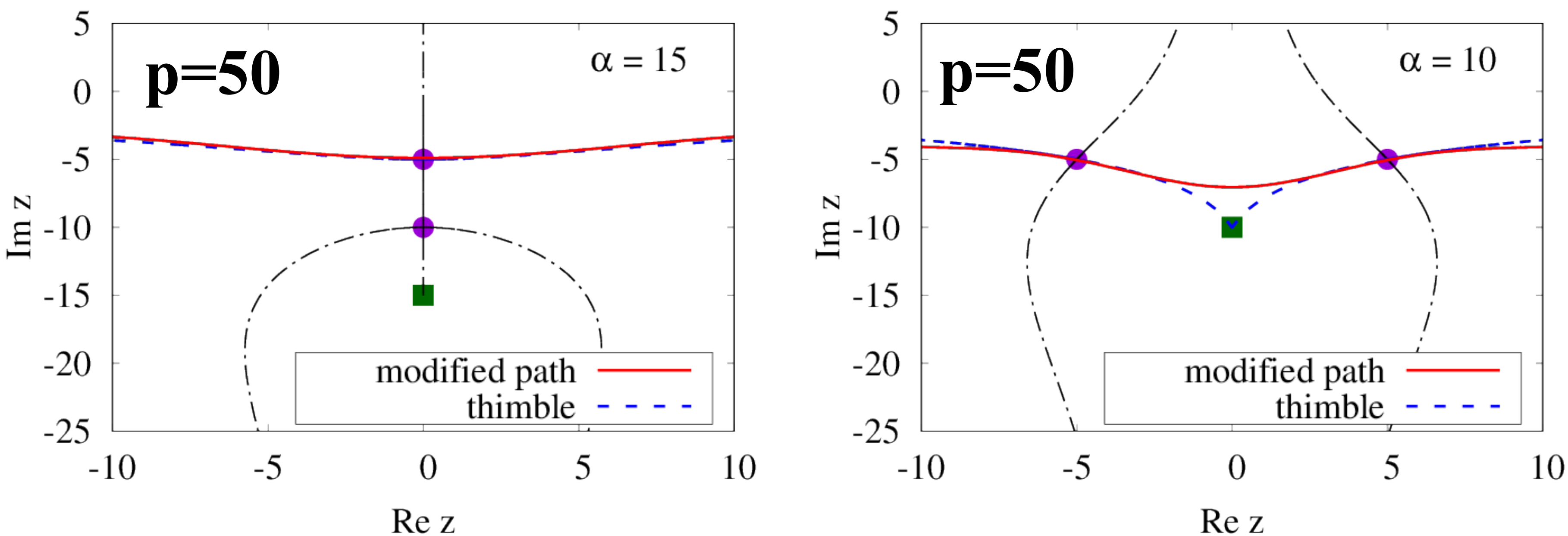
Optimized Path

Mori, Kashiwa, AO ('17)

- **Trial Function**

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

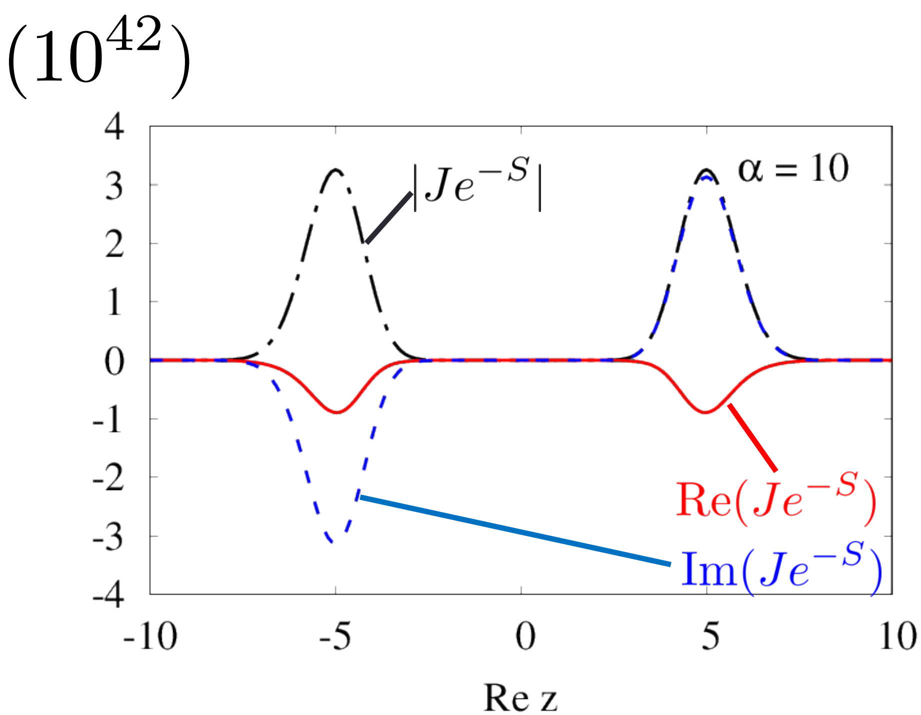
- **Optimization = Gradient descent**
- **Optimized path agrees with thimble(s) around the fixed point(s) !**
  - **Large α → One thimble, Singular point is far away from thimble**
  - **Small α → Go through two FPs.**

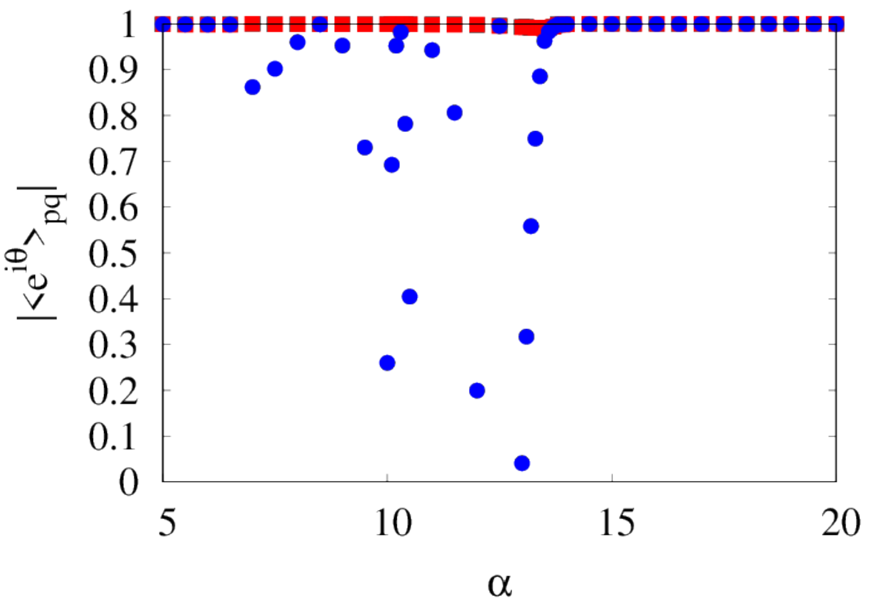


Average Phase Factor

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

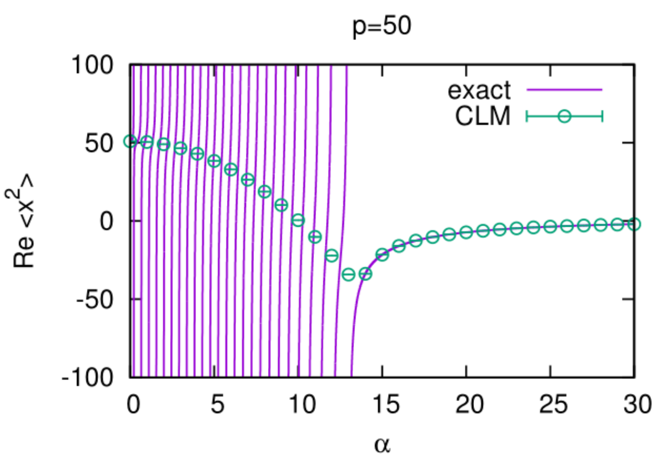
→ z=x+iy, -x+iy are sampled as a pair.
(or Exchange MC is necessary.)



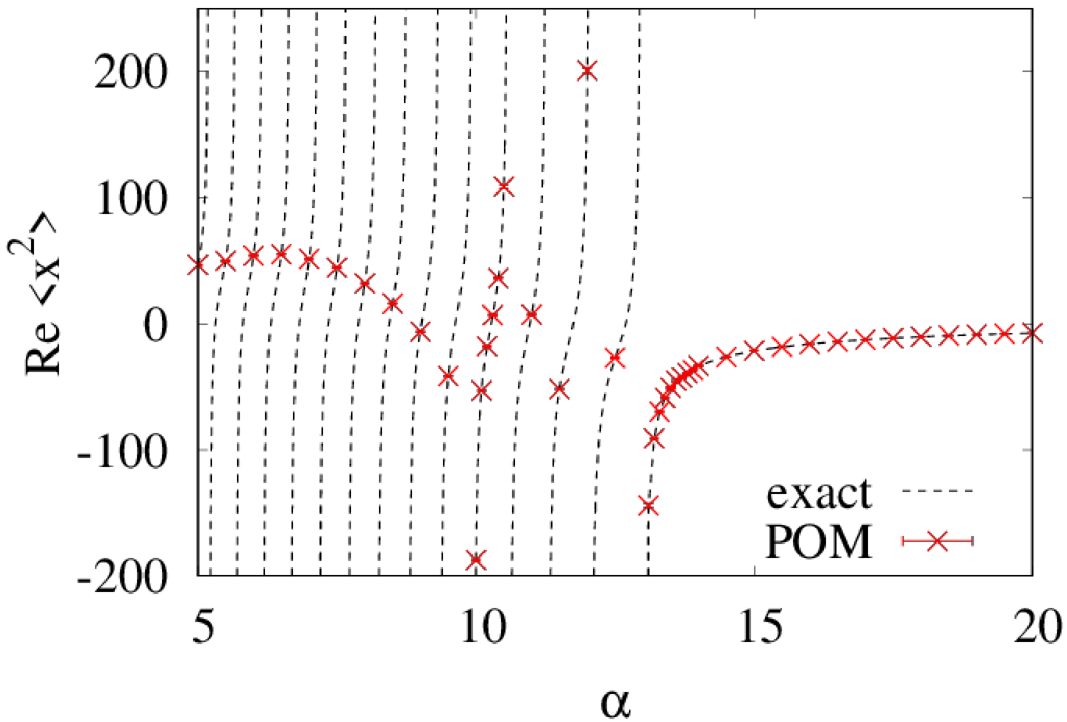


Expectation Value of x^2

- **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).**



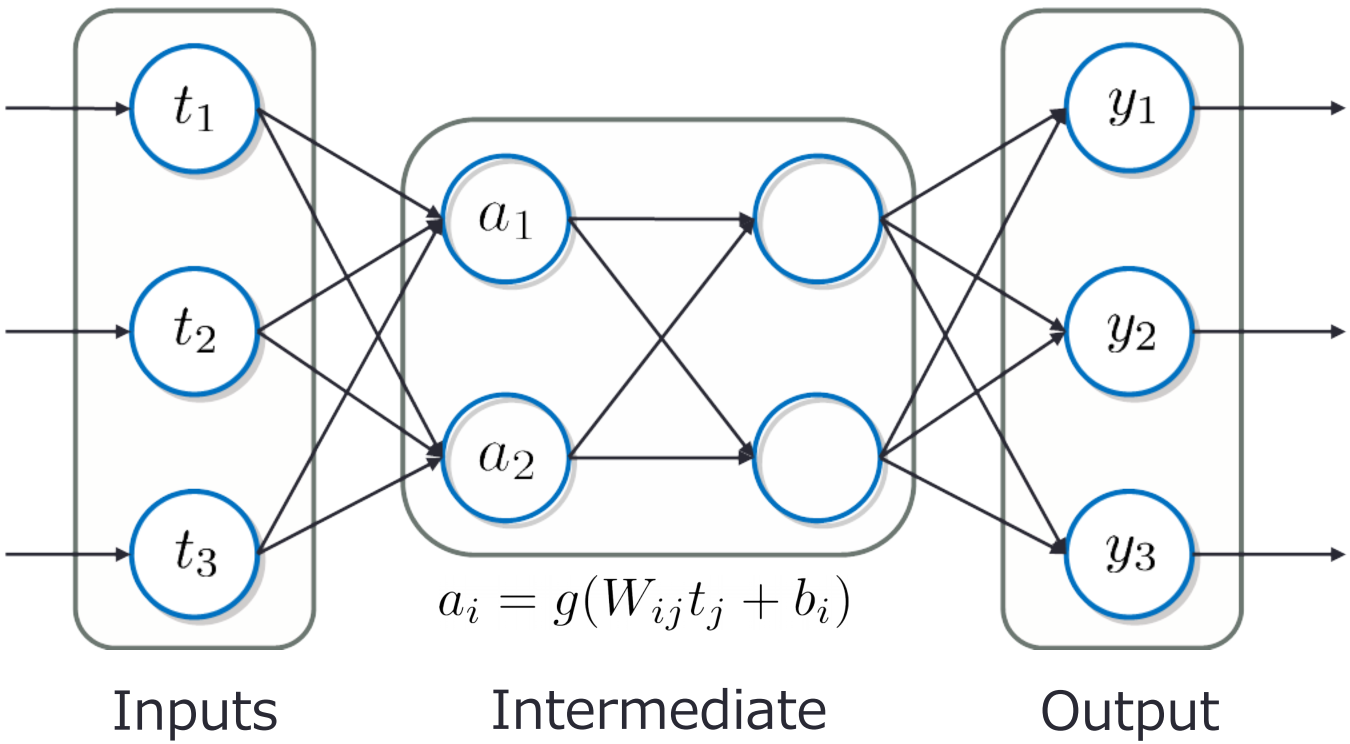
Nishimura, Shimasaki ('15)



Mori, Kashiwa, AO ('17)

Do we need to know the form of Trial Function ?

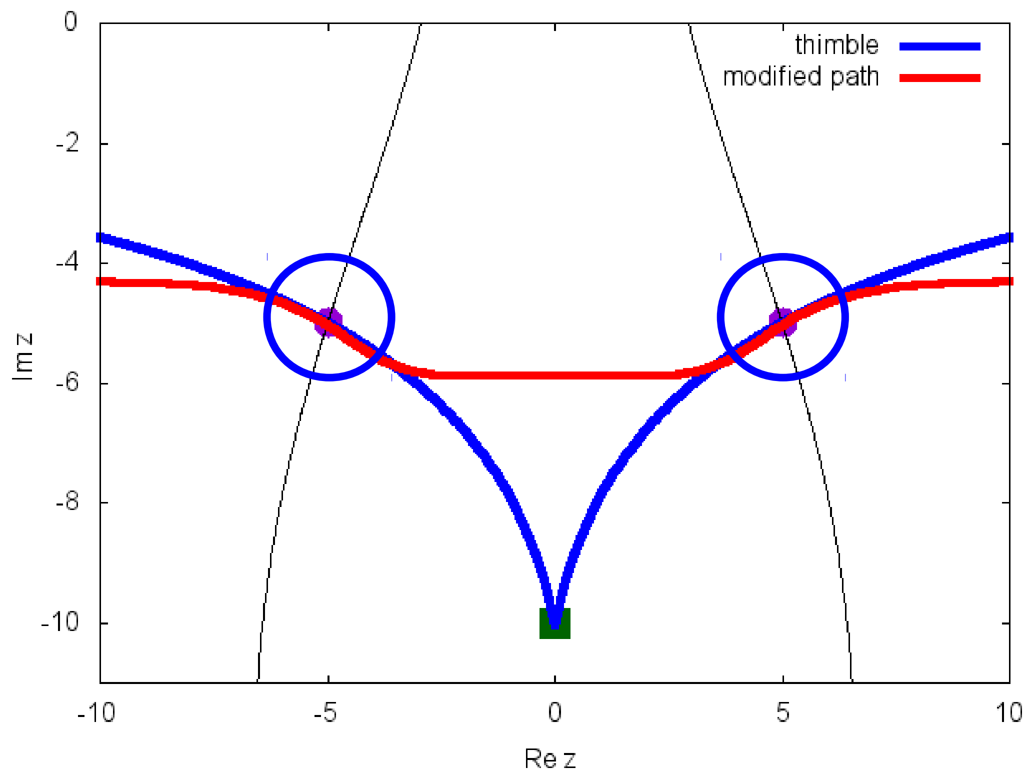
- **What happens for many variables ?**
  Trial fn. form, Variable corr., CPU cost, …
- **Neural Network**
  - **Combination of linear transf. + Non-linear network fn. g(x).**



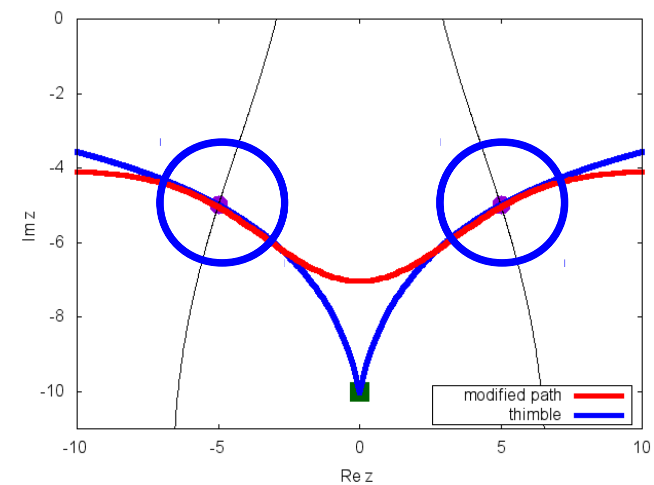
Mori, Kashiwa, AO (in prep.)

Optimized Path by Neural Network

Neural Network



Gaussian +Gradient Descent



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

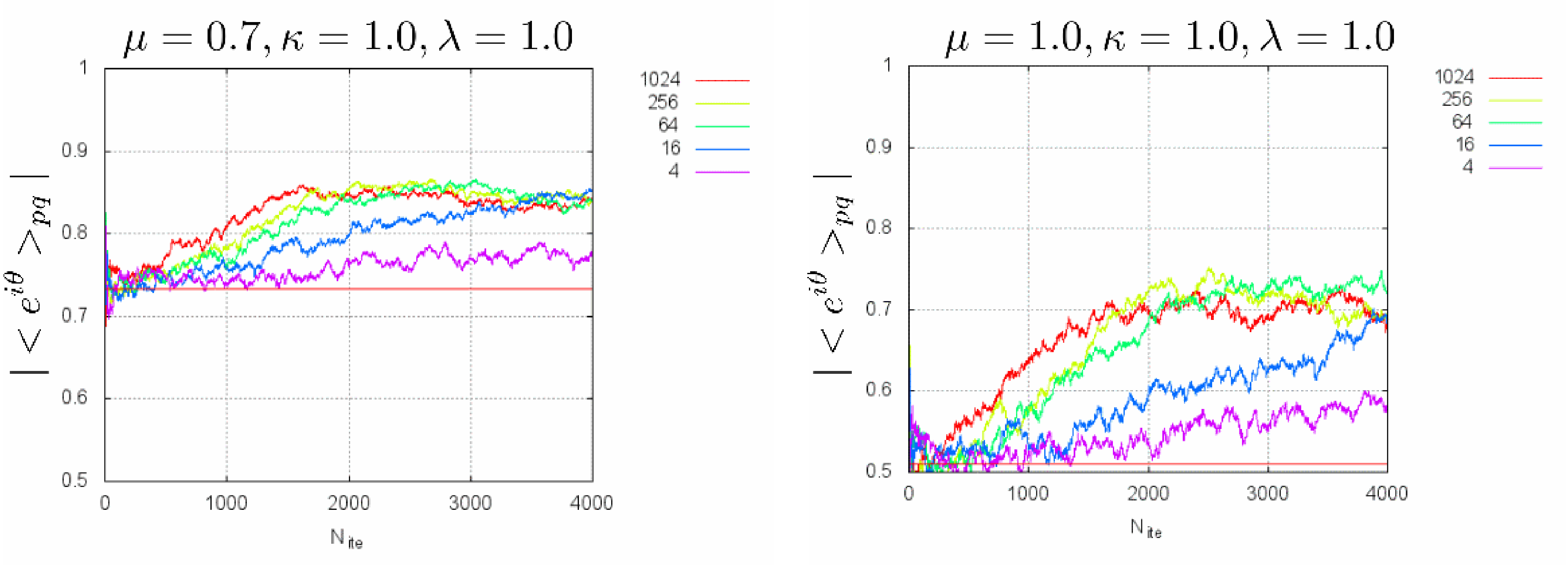
Mori, Kashiwa, AO (in prep.)

Summary

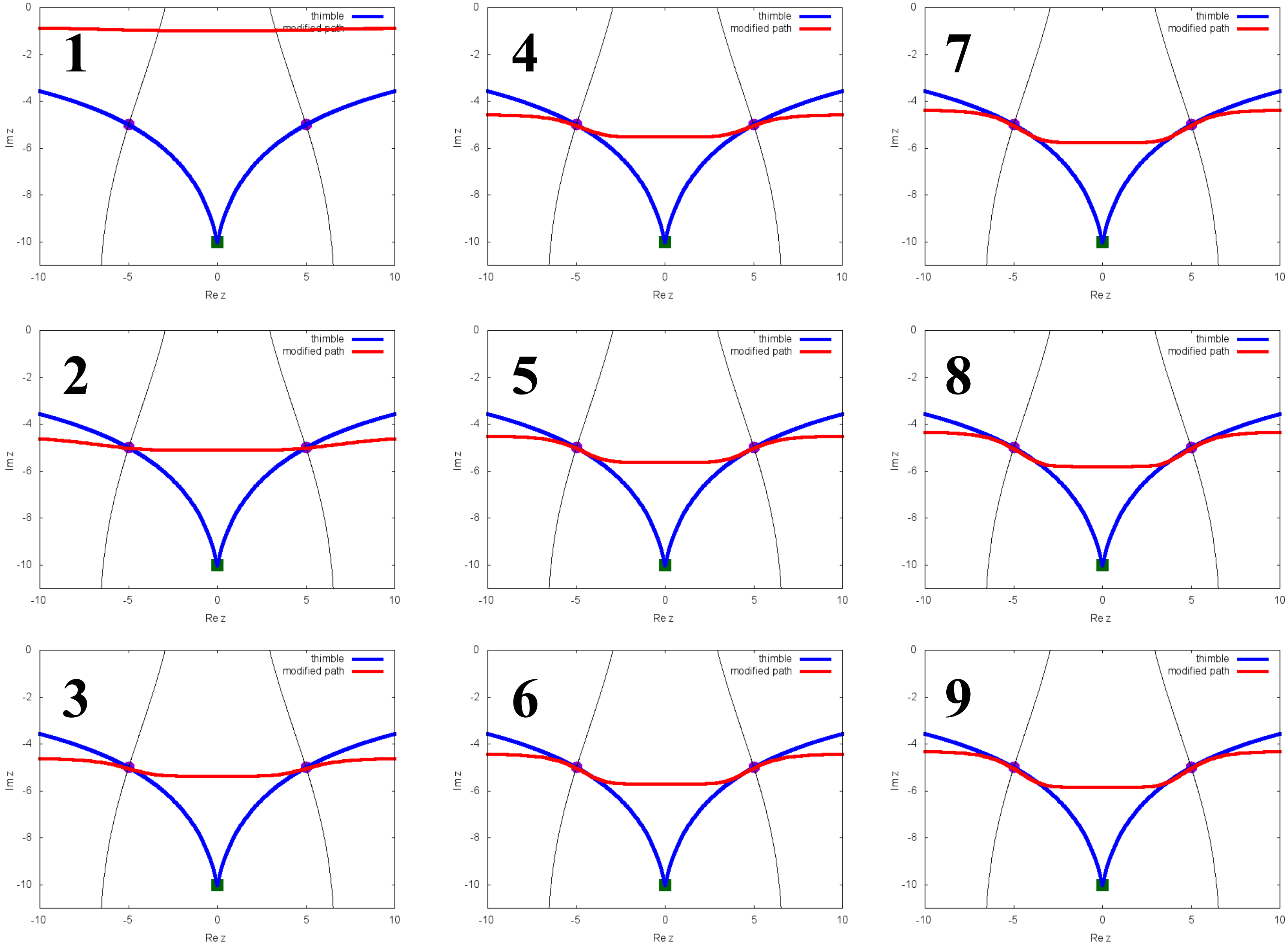
- Sign problem is a grand challenge in theoretical physics, and is relevant to dense QCD physics explored at J-PARC.
- Approaches to the sign problem have been improved rapidly, (Generalized) Lefshetz thimble, Complex Langevin, …, but flow equation and singularities are still problematics.
- Lefschetz thimbles in NJL (with many singular points) can be determined under the requirement of keeping the same Riemann sheet on the flow. Auxiliary sign problem may be solved by using thimbles.
- Path Optimization Method (POM) is proposed to tackle the sign problem. Integration path is optimized to reduce the cost function, and reproduces the thimble around the fixed points. It is possible to apply various optimization technique such as the neural network.

Application to Complex φ⁴ model

4x4 lattice

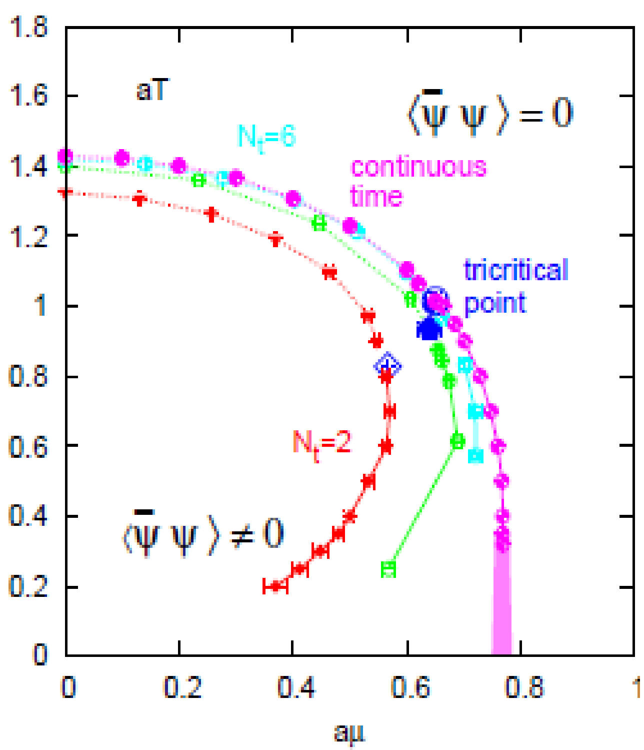


Optimized Path by Neural Network

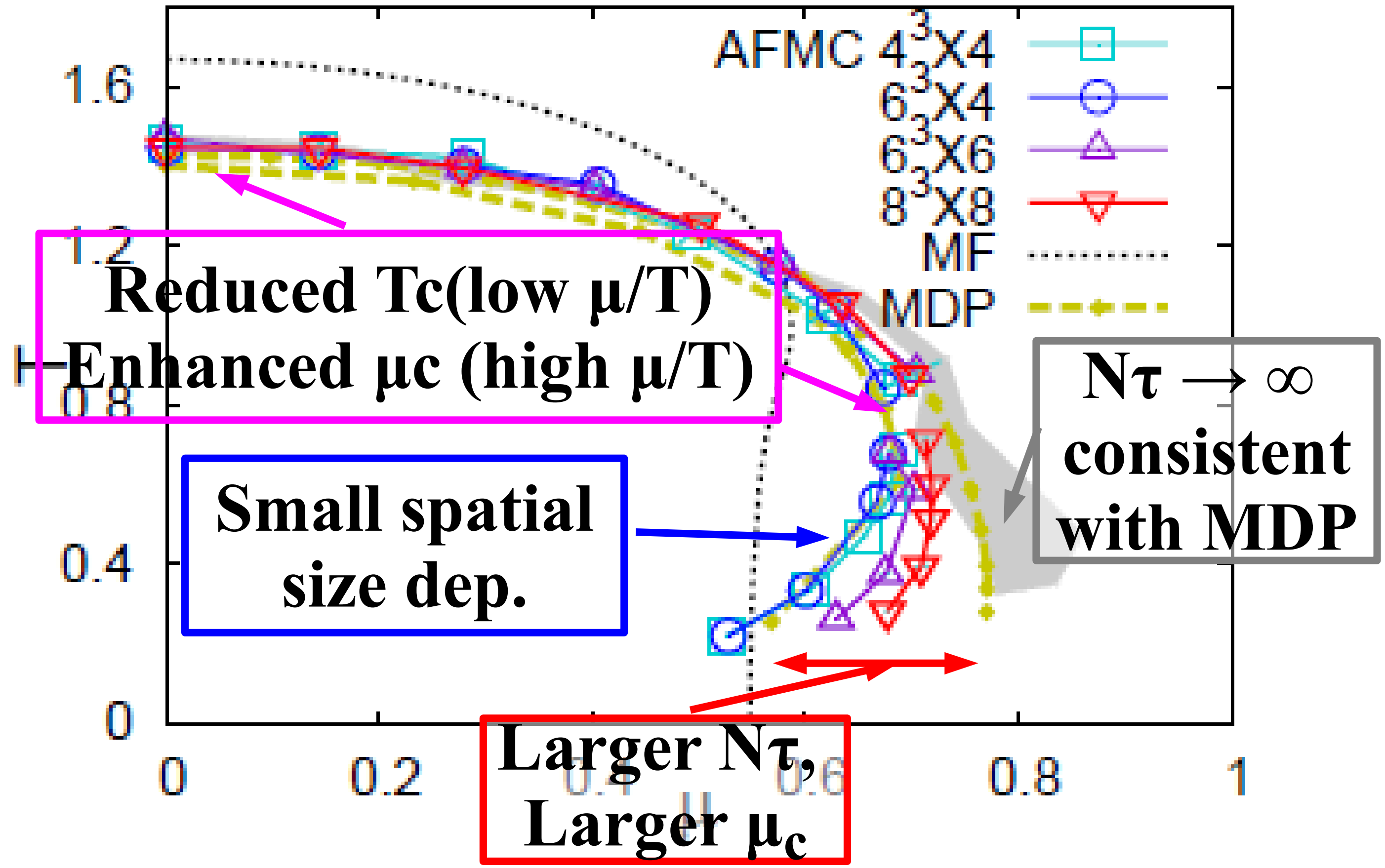


Phase diagram in the strong coupling limit

- **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)