Path optimization for the sign problem in low-dimensional QCD and QCD effective models at finite density

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Collaborators

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Y. Mori (PhD stu.)

K. Kashiwa

AO (11 yrs ago)

- *1D integral: Y. Mori, K. Kashiwa, AO, PRD 96 ('17), 111501(R) [arXiv:1705.05605]*
- *φ^4 w/ NN: Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [arXiv:1709.03208]*
- *Lat 2017: AO, Y. Mori, K. Kashiwa, EPJ Web Conf. 175 ('18), 07043 [arXiv:1712.01088]*
- *NJL thimble: Y. Mori, K. Kashiwa, AO, PLB 781('18),698 [arXiv:1705.03646]*
- *PNJL w/ NN: K. Kashiwa, Y. Mori, AO, PRD 99 ('19), 014033 [arXiv:1805.08940 [hep-ph]*
- *PNJL with vector int. using NN: K. Kashiwa, Y. Mori, AO, arXiv:1903.03679 [hep-lat]*
- *0+1D QCD: Y. Mori, K. Kashiwa, AO, in prep; AO, Y. Mori, K. Kashiwa, arXiv:1812.11506 (Lat2018 proc.)*

The Sign Problem

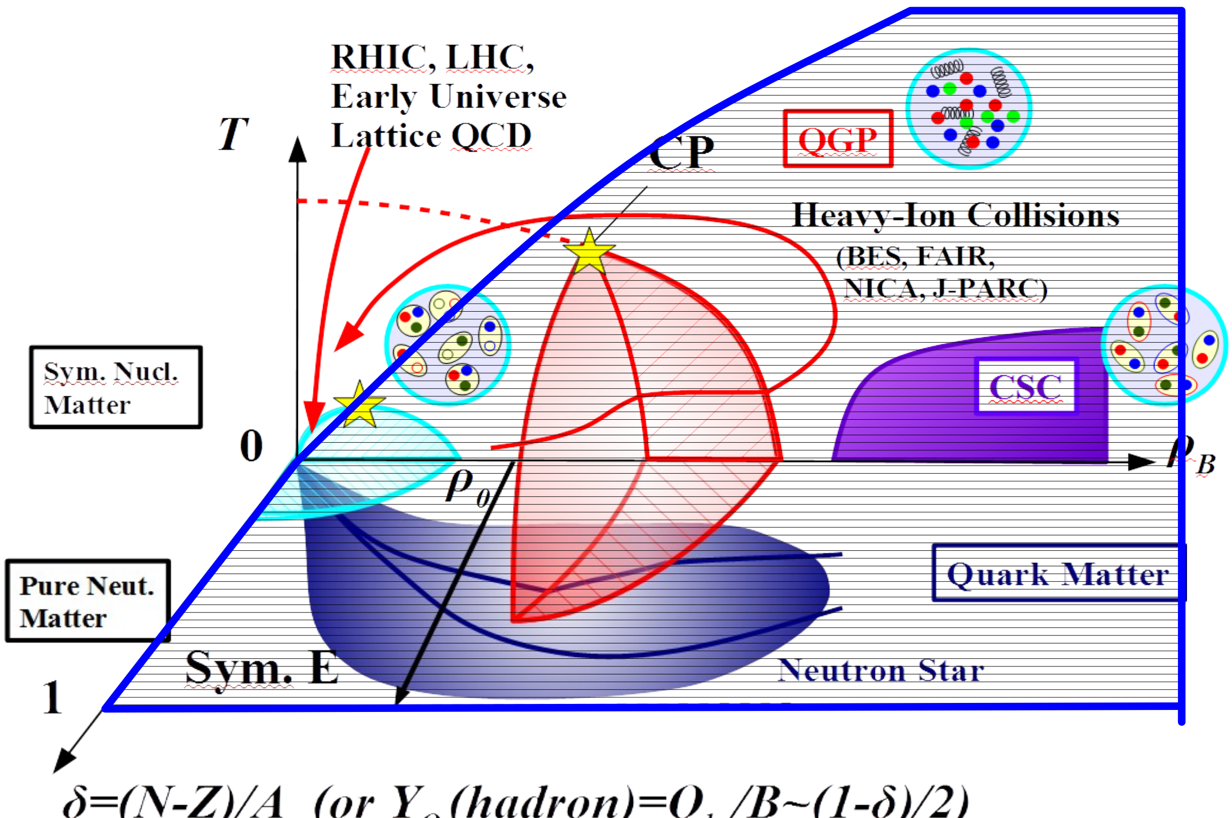
- **When the action is complex, strong cancellation occurs in the Boltzmann weight at large volume. = The Sign Problem**

$$\mathcal{Z} = \int \mathcal{D}x\, e^{-S(x)},\ |\mathcal{Z}| \ll \mathcal{Z}_{\rm pq} = \int \mathcal{D}x \left| e^{-S(x)} \right| \ \text{(at large } V\text{)}$$

- **Fermion det. is complex at finite density**

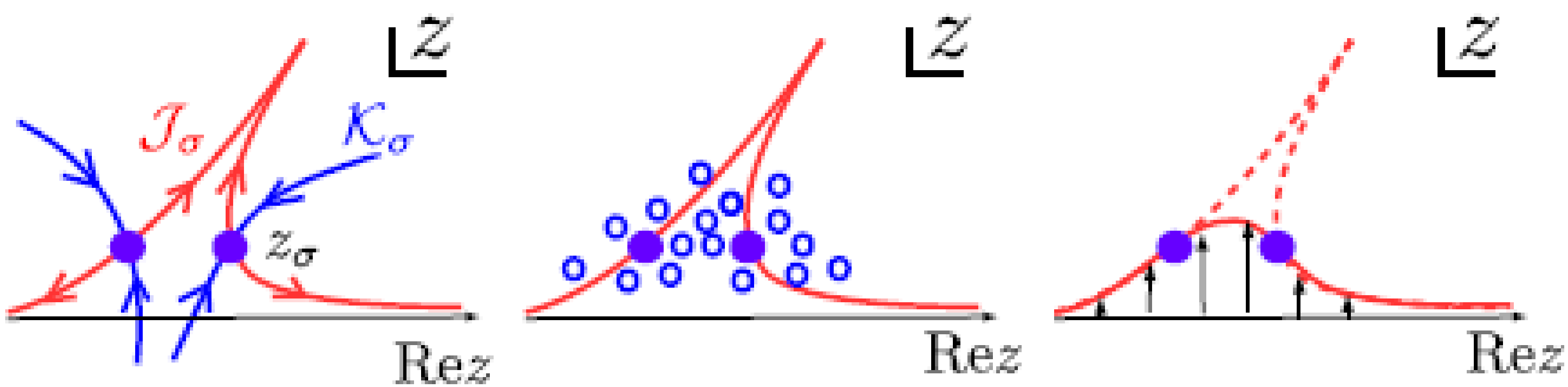
$$\det D(\mu) = (\det D(-\mu^*))^* \to S_{\rm eff} = S_{\rm boson} - \log\det D \in \mathbb{C}$$

- **Difficulty in studying finite density in LQCD**
  → Heavy-Ion Collisions, Neutron Star, Binary Neutron Star Mergers, Nuclei, …



Approaches to the Sign Problem

- **Standard approaches**
  - **Taylor exp., Imag. μ (Analytic cont. / Canonical), Strong coupling**
- **Integral in Complexified variable space**
  - **Lefschetz thimble method**
    Witten ('10), Cristoforetti+ (Aurora) ('12), Fujii+ ('13), Alexandru+ ('16).
  - **Complex Langevin method**
    Parisi ('83), Klauder ('83), Aarts+ ('11), Nagata+ ('16); Seiler+ ('13), Ito+ ('16).
  - **Path optimization method**
    Mori, Kashiwa, AO ('17,'18,'19); Kashiwa, Mori, AO ('18,19); AO, Mori, Kashiwa ('18,'19); Alexandru+('18), Bursa, Kroyter ('18)



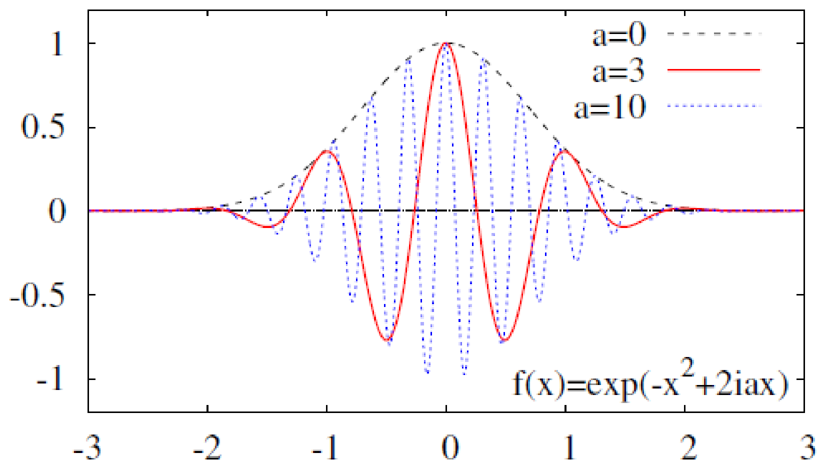
Lefshetz thimble **Complex Langevin** **Path Optimization**

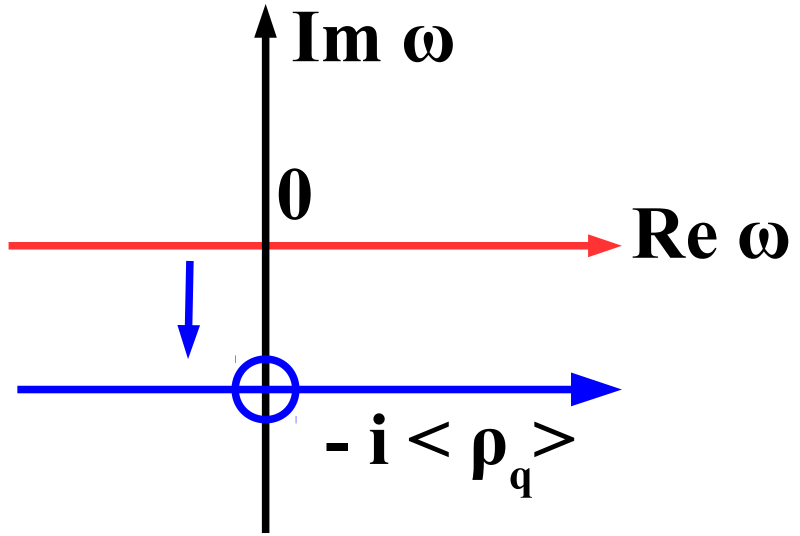
Integral in Complexified Variable Space

- **Simple Example: Gaussian integral (bosonized repulsive int.)**
  Mori, Kashiwa, AO ('18b)

$$\int_{\mathbb{R}} d\omega\, e^{-\omega^2/2 - i\omega\rho_q} = \int_{\mathbb{R}+i\rho_q} d\omega\, e^{-\underbrace{(\omega+i\rho_q)}_{z}{}^2/2-\rho_q^2/2}$$

$$= \exp(-\rho_q^2/2) \int_{\mathbb{R}} dz\, e^{-z^2/2}$$





Complexified variable methods
= Extension of the saddle point integral

Lefschetz thimble & Complex Langevin methods

- **Lefschetz thimble method**
  Witten ('10), Cristoforetti+ (Aurora) ('12), Fujii+ ('13), Alexandru+ ('16).
  - **Flow eq. from a fixed point σ → thimble (Im(S)=const.)**

$$\mathcal{J}_\sigma : \frac{dz_i(t)}{dt} = \overline{\left(\frac{\partial S}{\partial z_i}\right)} \to \frac{dS}{dt} = \sum_i \left|\frac{\partial S}{\partial z_i}\right|^2 \in \mathbb{R}, \quad \mathcal{C} = \sum_\sigma n_\sigma \mathcal{J}_\sigma$$

  - **Problems:Phase of Jacobian, Multimodal prb., Stokes phenomena, …**

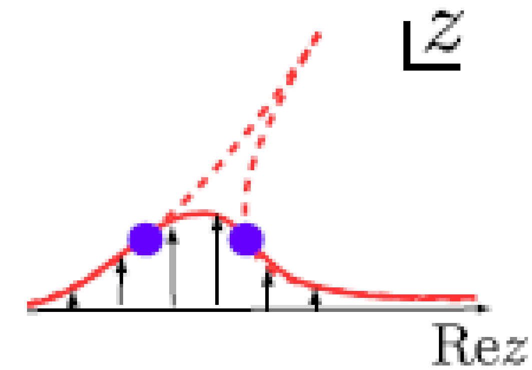
- **Complex Langevin method**
  Parisi ('83), Klauder ('83), Aarts+ ('11), Nagata+('16); Seiler+ ('13), Ito+ ('16).
  - **Complex Langevin eq.→ Configs.**

$$\frac{dz_i}{dt} = -\frac{\partial S}{\partial z_i} + \eta_i(t) (\eta_i : \text{White noize}),\ \langle \mathcal{O}(x) \rangle = \langle \mathcal{O}(z) \rangle$$

  - **Problems: Wrong conversion, Boundary terms, ...**

Path optimization method

Mori, Kashiwa, AO ('17,'18,'19); Kashiwa, Mori, AO ('18,19);
AO, Mori, Kashiwa ('18,'19); Alexandru+('18), Bursa, Kroyter ('18)



Path Optimization

- **Integration path is optimized to evade the sign problem, i.e. to enhance the average phase factor.**

$$\mathrm{APF} = \langle e^{i\theta} \rangle_{\mathrm{pq}} = \int dx e^{-S} / \int dx |e^{-S}| = \mathcal{Z}/\mathcal{Z}_{\mathrm{pq}}$$

Sign Problem → Optimization Problem

- **Cauchy(-Poincare) theorem: the partition fn. is invariant if**
  - **the Boltzmann weight W=exp(-S) is holomorphic (analytic), and the path does not go across the poles and cuts of W.**
- **S is singular but W is not singular when fermion det.=0.**

Application of POM to Field Theory

- **Cost function: a measure of the seriousness of the sign problem.**

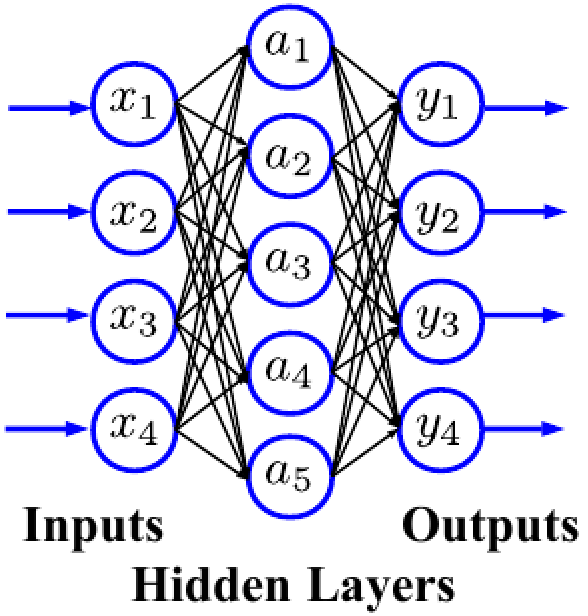
$$\mathcal{F}[z(x)] = |\mathcal{Z}| \left(\left| \langle e^{i\theta} \rangle_{\rm pq} \right|^{-1} - 1 \right)$$

- **Optimization: Gradient Descent or Neural Network**
  - **Neural network = Combination of linear and non-linear transf.**

$$a_i = g(\underline{W_{ij}^{(1)}} x_j + \underline{b_i^{(1)}})$$
$$f_i = g(\underline{W_{ij}^{(2)}} a_j + \underline{b_i^{(2)}})$$
$$z_i = x_i + i(\underline{\alpha_i} f_i(x) + \underline{\beta_i})$$
$$g(x) = \tanh x \ \text{(activation fn.)}$$

variational parameters

  - **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

Grad. Desc. :

$$dc_i/dt = -\partial\mathcal{F}/\partial c_i$$

par. in (j+1)th step → $c_i^{(j+1)}$

Learning rate → η

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

mean sq. ave. of v → $s_i^{(j)}$

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

decay rate → γ

mean sq. ave. of F → $r_i^{(j+1)}$

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

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

gradient evaluated in MC (batch training) → F_i

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

Cost fn. → $\mathcal{F}$

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

Hybrid Monte-Carlo with Neural Network

Initial Config. on Real Axis

HMC $H(x,p) = \frac{p^2}{2} + \mathrm{Re}S(z(x))$

Jacobian
→ via Metropolis judge

Do k = 1, Nepoch
Do j = 1, Nconf/Nbatch

Mini-batch training of Neural Network

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

Grad. wrt parameters (Nbatch configs.)

$F_i = \frac{1}{N_{\mathrm{batch}}} \sum_n \partial\mathcal{F}(n)/\partial c_i$

New Nbatch configs. by HMC

$H(x,p) = \frac{p^2}{2} + \mathrm{Re}S(z(x))$

Enddo
Enddo

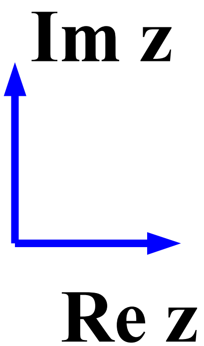
Nbatch ~ 10, Nconfig ~ 10,000, Nepoch ~ (10-20)

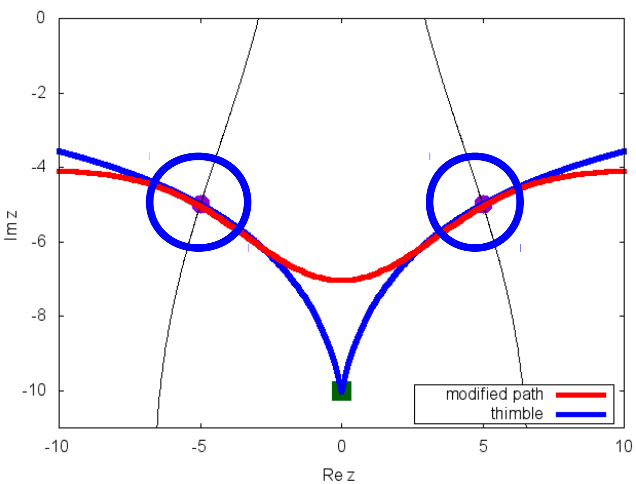
Benchmark test (1): 1 dim. integral

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

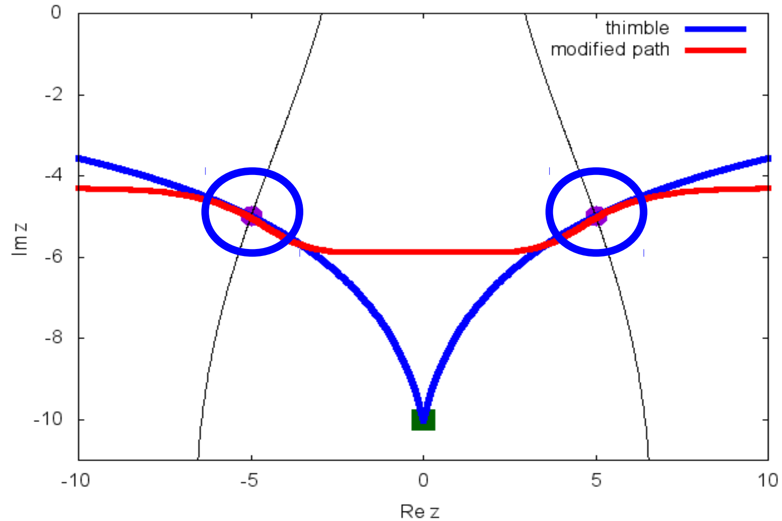
J. Nishimura, S. Shimasaki ('15)

Gaussian+Gradient Descent

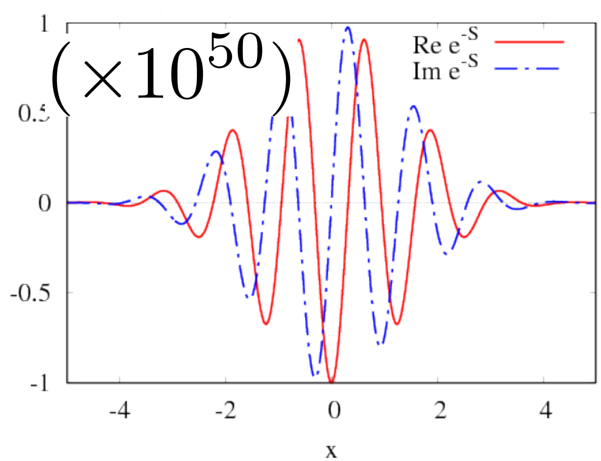




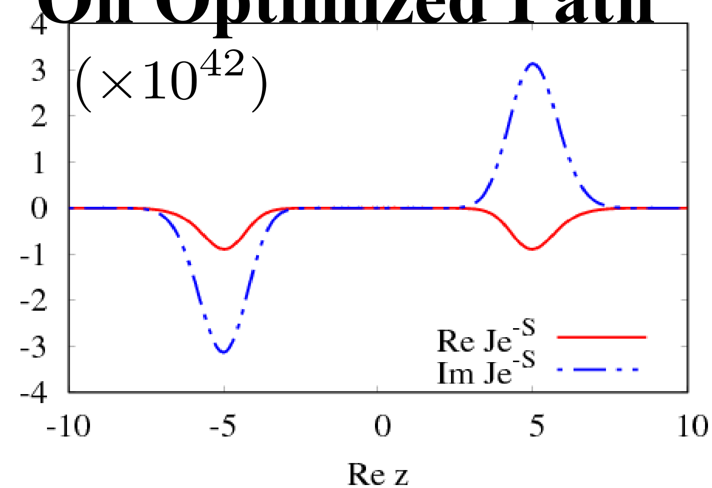
Neural Network



On Real Axis



On Optimized Path



Mori, Kashiwa, AO ('17); AO, Mori, Kashiwa (Lat 2017)

Benchmark test (2): Complex φ^4 theory at finite μ

- **Complex Langevin & Lefschetz thimble work.**
  G. Aarts, PRL102('09)131601; H. Fujii, et al., JHEP 1310 (2013) 147

- **How about POM ?**
  - **1+1D Complex φ^4 theory**
    Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [arXiv:1709.03208]

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

$$S = \sum_x \left[\frac{(4+m^2)}{2} \phi_{a,x}\phi_{a,x} + \frac{\lambda}{4} (\phi_{a,x}\phi_{a,x})^2 - \phi_{a,x}\phi_{a,x+\hat{1}} - \cosh\mu\, \phi_{a,x}\phi_{a,x+\hat{0}} + \underbrace{i\epsilon_{ab} \sinh\mu\, \phi_{a,x}\phi_{b,x+\hat{0}}}_{\text{complex}} \right]$$

complex

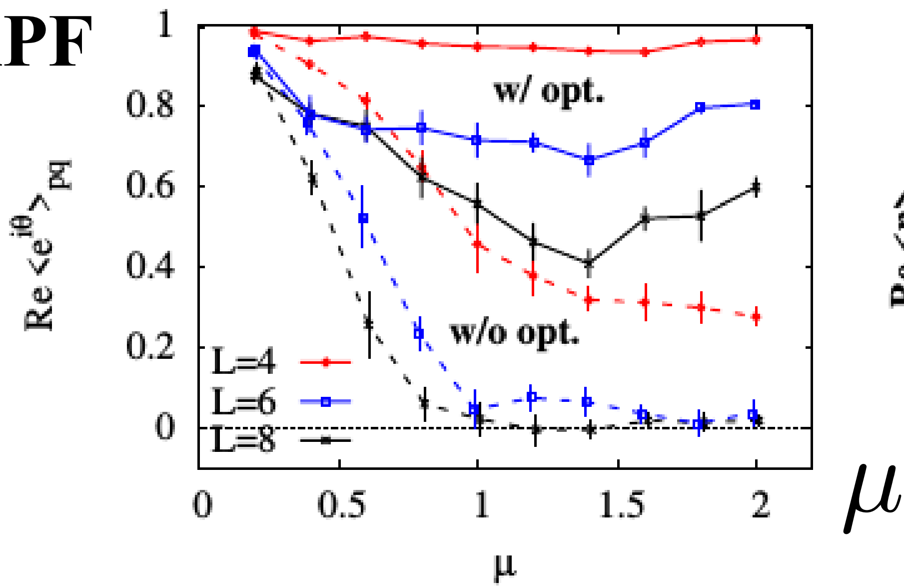
$$\left(\phi = \frac{1}{\sqrt{2}} (\underline{\phi_1} + i \underline{\phi_2}) \right)$$

Complexify

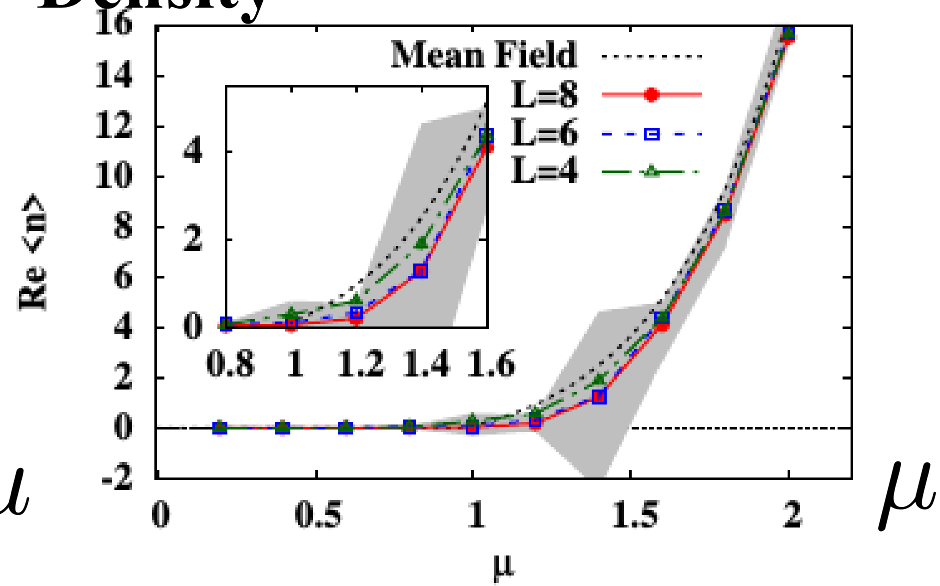
POM in 1+1D φ⁴ theory

- **POM for 1+1D φ^4 theory**
  Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [arXiv:1709.03208]
  - **4^2, 6^2, 8^2 lattices, λ=m=1**
  - **$\mu_c \sim 0.96$ in the mean field approximation**

APF



Density



> ***POM also works !***
> - ***Enhancement of the APF after optimization.***
> - ***Density is suppressed at μ < m. (Silver Blaze)***

Path Optimization Method w/ Neural Network seems to work in 1D integral and simple field theories.

How about gauge theory ?
What happens when phase transition occurs ?

Contents

- **Introduction of Path Optimization Method**

  Y. Mori, K. Kashiwa, AO, PRD 96 ('17), 111501(R) [1705.05605]
  Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [1709.03208]
  AO, Y. Mori, K. Kashiwa, EPJ Web Conf. 175 ('18), 07043 [1712.01088](Lat 2017)

- **Application to gauge theory: 1-dimensional QCD**

  Mori, K Kashiwa, AO, in prep.
  AO, Y. Mori, K. Kashiwa, PoS LATTICE2018 ('19), 023 (1-15) [1812.11506]

- **Application to QCD effective models**

  K. Kashiwa, Y. Mori, AO, PRD99('19)014033 [1805.08940]
  K. Kashiwa, Y. Mori, AO, arXiv:1903.03679 [hep-lat]

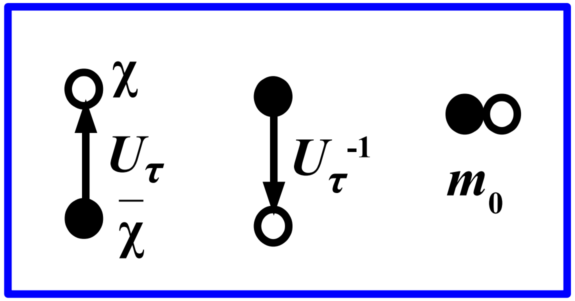
- **Discussions**
- **Summary**

Application to Gauge Theory: 1 dimensional QCD

0+1 dimensional QCD

- **0+1 dimensional QCD (1 dim. QCD) with one species of staggered fermion on a 1xN_τ lattice**

$$S = \frac{1}{2}\sum_\tau \left(\bar{\chi}_\tau e^{\mu} U_\tau \chi_{\tau+\hat{0}} - \bar{\chi}_{\tau+\hat{0}} e^{-\mu} U_\tau^{-1} \chi_\tau\right) + m\sum_\tau \bar{\chi}_\tau \chi_\tau = \frac{1}{2}\bar{\chi} D \chi$$



Bilic+('88), Ravagli+('07), Aarts+('10, CLM), Bloch+('13, subset), Schmidt+('16, LTM), Di Renzo+('17, LTM)

  - **A toy model, but includes the actual source of 3+1D QCD sign prob.**
  - **Reduces to a diagonalized one-link problem.**

$$\mathcal{Z} = \int dU e^{-S} = \int dx_1 dx_2 J \underbrace{\left[\frac{8}{3\pi^2}\prod_{a<b}\sin^2\left(\frac{z_a - z_b}{2}\right)\right]}_{\text{Haar measure}} \underbrace{\left[\prod_a (X_N + 2\cos(z_a - i\mu)\right]}_{\text{exp(-S)}}$$

Haar measure **exp(-S)**

→ Analytic results are known.

Fermion determinant in 1 dim. QCD

- **Fermion determinant (Temporal gauge) reduces to Nc x Nc det.**

$$D = \begin{pmatrix} I_1 & e^{\mu} & 0 & & e^{-\mu}U^{-1} \\ -e^{-\mu} & I_2 & e^{\mu} & & \\ 0 & -e^{-\mu} & I_3 & e^{\mu} & \\ \vdots & & & \ddots & \\ -e^{\mu}U & & & -e^{-\mu} & I_N \end{pmatrix} \quad N_c \times N_\tau \qquad X = \begin{vmatrix} I_1 & e^{\mu} & 0 & & 0 \\ -e^{-\mu} & I_2 & e^{\mu} & & \\ 0 & -e^{-\mu} & I_3 & e^{\mu} & \\ \vdots & & & \ddots & \\ 0 & & & -e^{-\mu} & I_N \end{vmatrix}$$

$$\det D = \det \left[X \otimes 1_c + (-1)^{N_\tau} e^{\mu/T} U + e^{-\mu/T} U^{-1} \right] \quad N_c \qquad I_k = 2m_q(\boldsymbol{x}, \tau_k)$$

- **For constant σ, *X* is obtained as**

$$X = 2\cosh(E/T)$$

$$E = \mathrm{arcsinh}\, m_q$$

$$\to \int dU \det D = \frac{\sinh[(N_c + 1)E/T]}{\sinh(E/T)} + 2\cosh(N_c\mu/T)$$

Faldt, Petersson ('86)

Partition Function in 1 dim. QCD

- **Partition Function**

$$D = X + e^{\mu/T} U + e^{-\mu/T} U^{-1}$$

$$\mathcal{Z} = \int dU \, \det D(U) = \frac{\sinh[(N_c+1)E/T]}{\sinh(E/T)} + 2\cosh(N_c \, \mu/T)$$

$$= X^3 - 2X + 2\cosh(N_c \, \mu/T) \quad (N_c = 3)$$

$$\det D = X^3 + N_c X (N_c \overline{P}_U P_U - 1) + 2\cosh(N_c \mu/T)$$
$$+ N_c X^2 (e^{\mu/T} P_U + e^{-\mu/T} \overline{P}_U) + N_c X (e^{2\mu/T} \overline{P}_U + e^{-2\mu/T} P_U)$$
$$+ N_c e^{\mu/T} (N_c \overline{P}_U^2 - 2P_U) + N_c e^{-\mu/T} (N_c P_U^2 - 2\overline{P}_U)$$
$$\left(N_c = 3, P_U = \mathrm{tr} U / N_c, \int dU \overline{P}_U P_U = 1/N_c^2\right)$$

- **Chiral condensate, Quark number density, Polyakov loop**

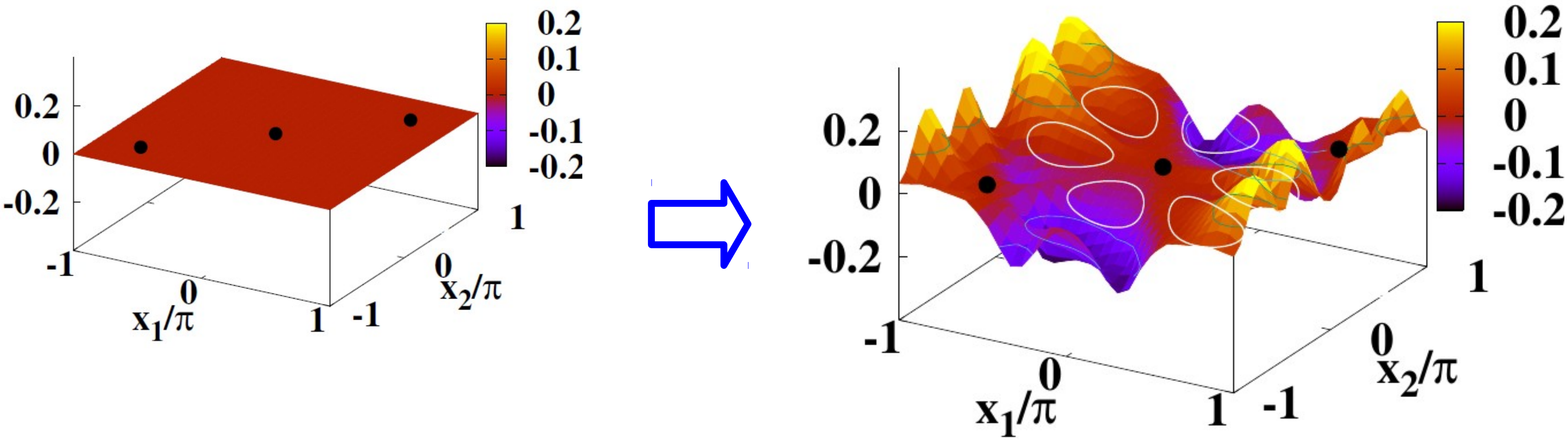
$$\sigma = \frac{T}{V} \frac{\partial}{\partial m} \log Z, \quad n_q = -\frac{T}{V} \frac{\partial}{\partial \mu} \log Z$$

$$P = \left\langle \frac{1}{N_c} \mathrm{Tr}\, U \right\rangle = \frac{1}{N_c} \frac{(X^2 - 1) e^{-\mu/T} + X e^{2\mu/T}}{X^3 - 2X + 2\cosh(3\mu/T)}$$

Faldt, Petersson ('86)
Bilic, Demeterfi ('88)

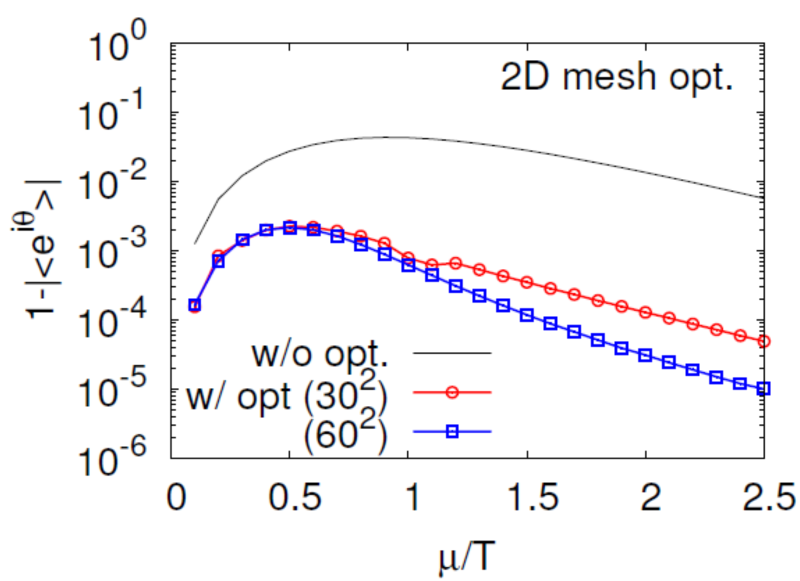
1 dim. QCD in diagonalized gauge (1)

- **2 variable problem → 2D mesh point integral**
  → $y_{1,2}(x_1,x_2)$ are variational parameters by themselves.



- **Average phase factor > 0.997**
  - **(Normal) gradient descent**
  - **Good enough for small lattice in 3+1D.**

$$(\mathrm{APF})_{0+1}^{L^3} \simeq 0.21(L=8)$$



Mori, Kashiwa, AO, in prep.

1 dim. QCD in diagonalized gauge (2)

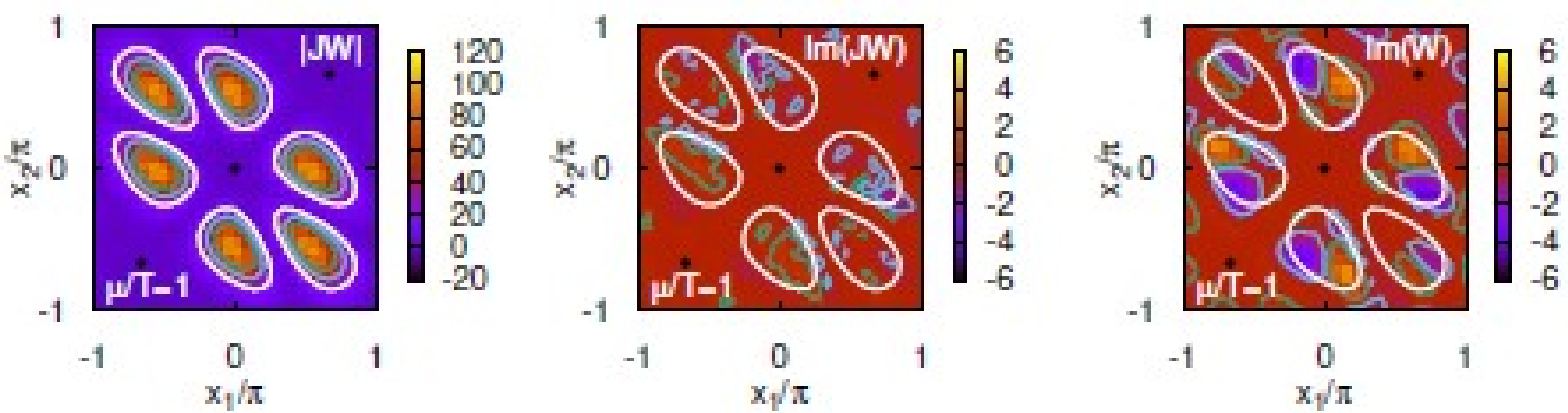
- **Jacobian is also important !**

$$|\mathrm{Im}(JW)| \ll |\mathrm{Im}W| \quad (W = H\exp(-S))$$

- **There are six regions with large stat. weight | *JW* |.**

$$\text{Symmetry}: \quad S(-z) = (S(z^*))^*, z_i \leftrightarrow z_j (i,j=1,2,3)$$

→ Problematic in sampling in Hybrid MC



Mori, Kashiwa, AO, in prep.

1 dim. QCD w/o diagonalized gauge fixing (1)

- **Complexification of link variable**

$$U \to \mathcal{U}(U) = U \prod_{a=1}^{N_c^2-1} e^{-y_i \lambda_i}$$

$$= U \boxed{e^{-y_1\lambda_1} e^{-y_2\lambda_2} \cdots e^{-y_8\lambda_8}} \in \mathrm{SL}(3)$$

  - **Derivative wrt y's is easy. Parametrization deps. is taken care by J.**

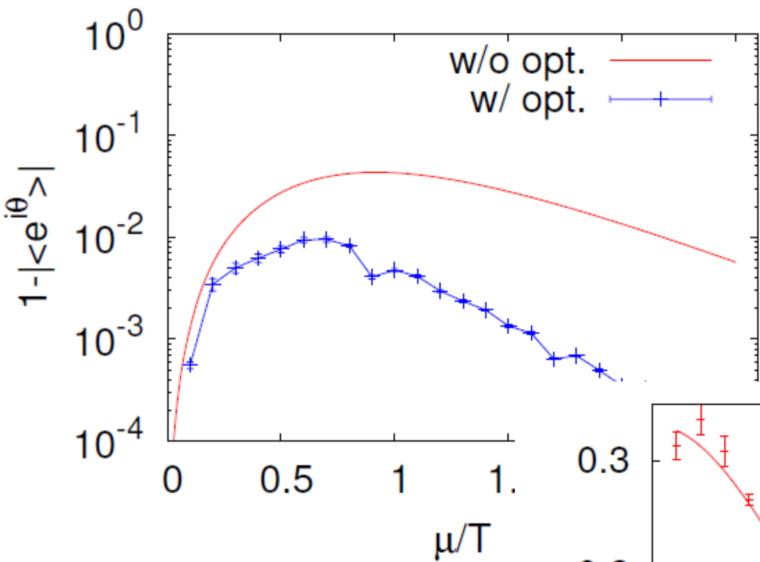
- **Hybrid Monte-Carlo in 1 dim. QCD**

$$H = \frac{P^2}{2} + \mathrm{Re}(S(\mathcal{U}(U)))$$

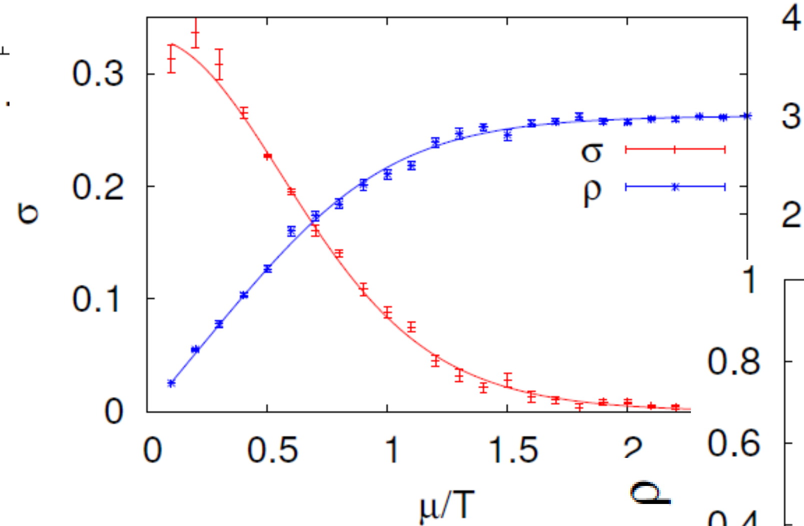
- **8 variables → path optimization using Neural Network**

1 dim. QCD w/o diagonalized gauge fixing (2)

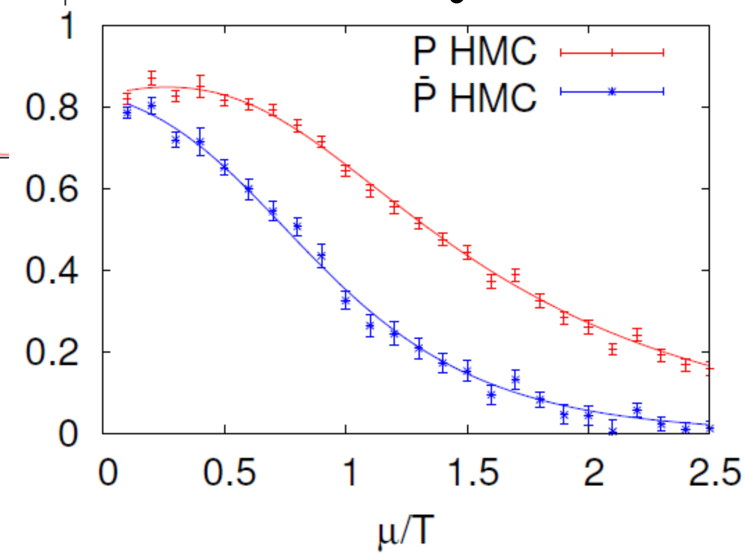
Average phase factor



Chiral condensate
& Quark number density



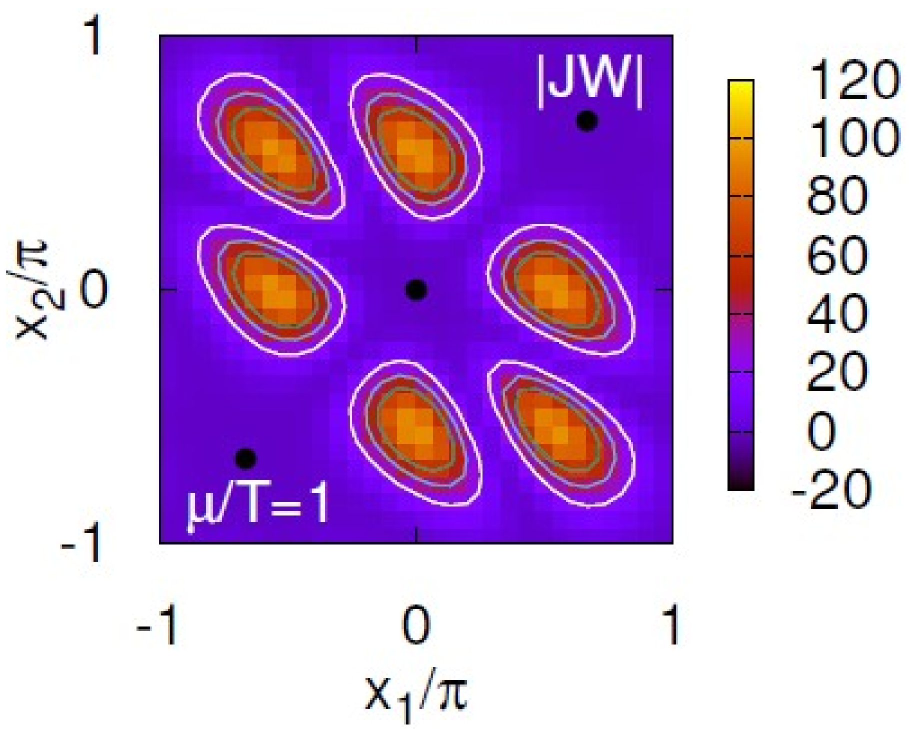
Polyakov loop

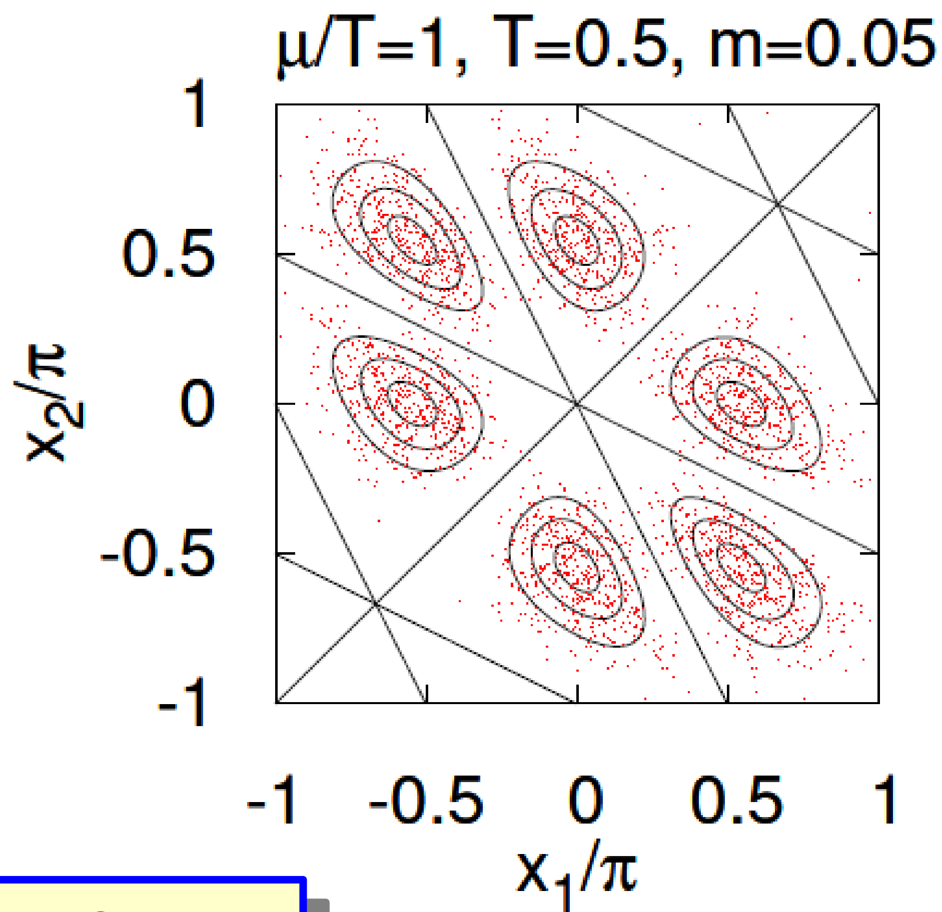


Mori, Kashiwa, AO, in prep.

1 dim. QCD w/o diagonalized gauge fixing (3)

- **Statistical weight distribution in diagonalized gauge ~ Config. dist. in Hybrid MC w/o diag. gauge fixing**





It would be possible to apply POM in more realistic cases !

Mori, Kashiwa, AO, in prep.

Application to QCD effective models

Polyakov-loop-extended NJL (PNJL) model

- **Sign problem is more severe around the phase boundary.**
  e.g. S. Tsutsui et al., 1811.07647; Y. Ito et al., 1811.12688.
  → Let us discuss QCD effecitve models !

- **Polyakov-loop-extended Nambu-Jona-Lasinio (PNJL) model with vector coupling**

$$\mathcal{L}_E = \bar{q}(\not{D} + m_0)q - G\left[(\bar{q}q)^2 + (\bar{q}i\gamma_5\boldsymbol{\tau}q)^2\right] + \underbrace{\mathcal{V}_g(\Phi, \bar{\Phi})}_{\text{Polyakov}} + \underbrace{G_v(\bar{q}\gamma_\mu q)^2}_{\text{Vector}}$$

- **Bosonizaiton & Truncation to homogeneous aux. field**

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

$$f^- = 1 + 3\Phi e^{-\beta E_p^-} + 3\bar{\Phi}e^{-2\beta E_p^-} + e^{-3\beta E_p^-}$$

$$E_p = \sqrt{p^2 + (m_0 - 2G\sigma)^2},\ E_p^\mp = E_p \mp \tilde{\mu},\ \tilde{\mu} = \mu - 2iG_v\omega$$

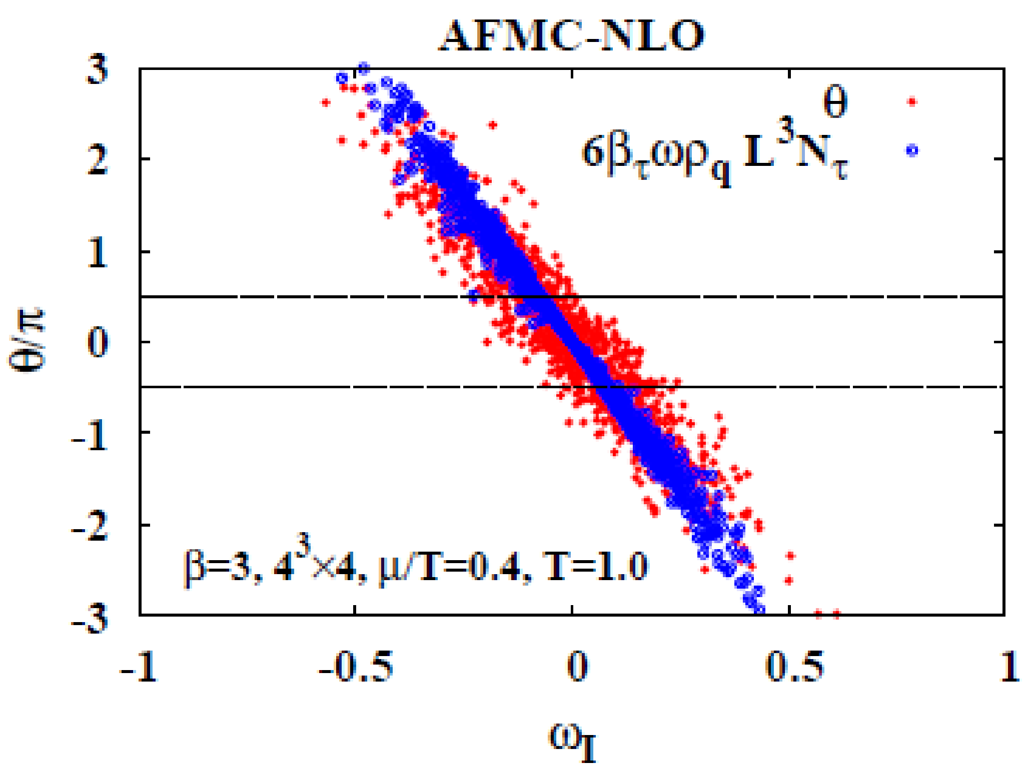
Φ, $\bar{\Phi}$, ω cause the sign prb.

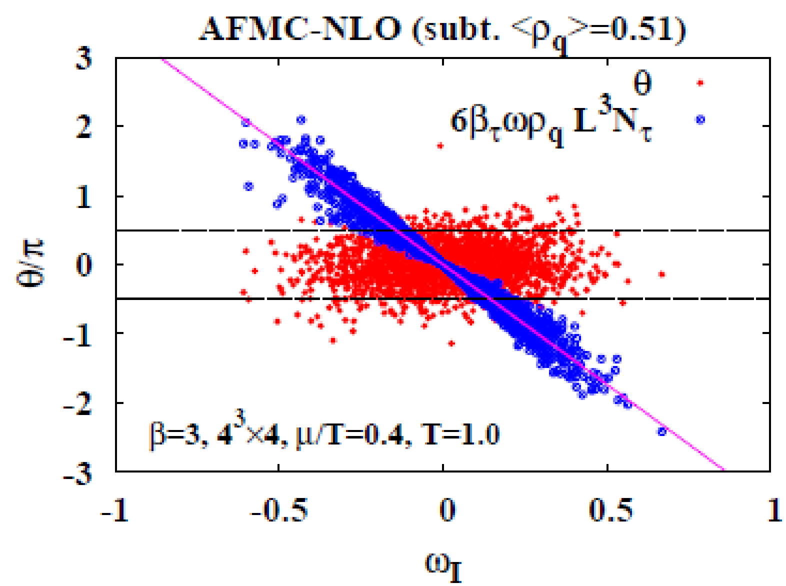
Repulsive interaction causes the sign problem

- **Hubbard-Stratonovich transformation of repulsive interaction**

$$\exp[-\alpha(\bar{q}\Gamma q)^2] = \int d\omega \exp[-\alpha\omega^2 + i\alpha\omega\bar{q}\Gamma q]$$

  - **This "model" sign problem causes trouble in Shell Model Monte-Carlo, Strong-coupling LQCD, …**





Complexification & Shift

AO, Ichihara (Lattice2015)

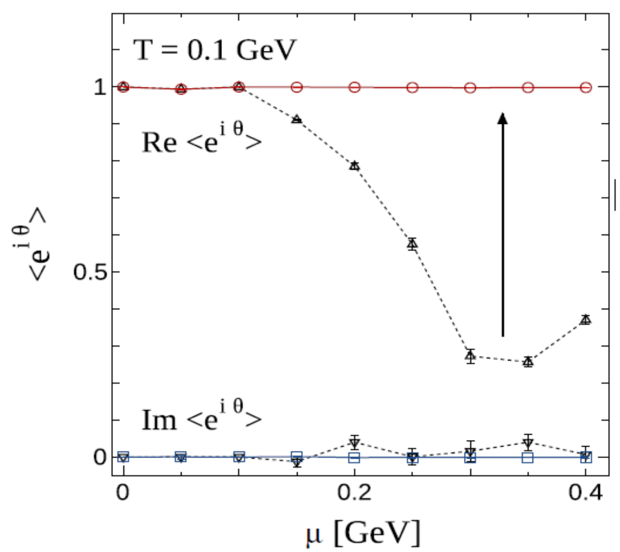
POM for PNJL (w/o vector coupling)

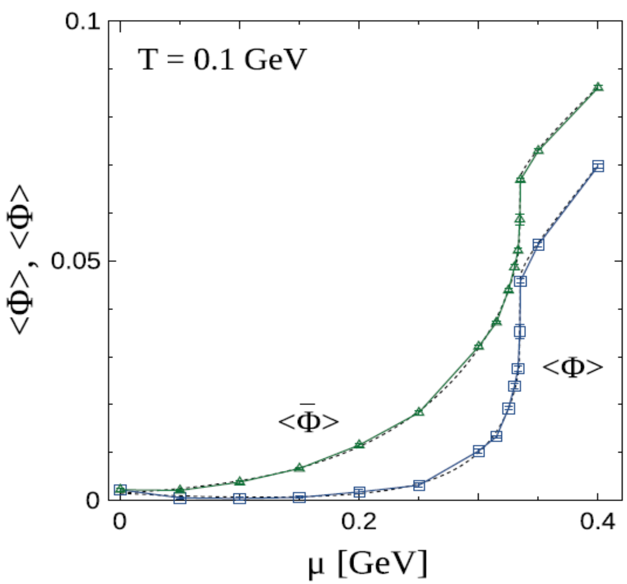
- **Partition function**

$$\mathcal{Z} = \int dX \exp(-\beta\mathcal{V}/V) = \int dX \exp(-k\mathcal{V}/T^4) \ (dX = dA_3 dA_8 d\sigma d\omega \ldots)$$

Homogenous field ansatz & const. k approx.
→ Results converge to mean field results at large k
Cristoforetti, Hell, Klein, Weise ('10) (MC-NJL)

- **POM works in PNJL !**
  - **Average phase factor ~ 1, Pol. loop converges to MF results.**

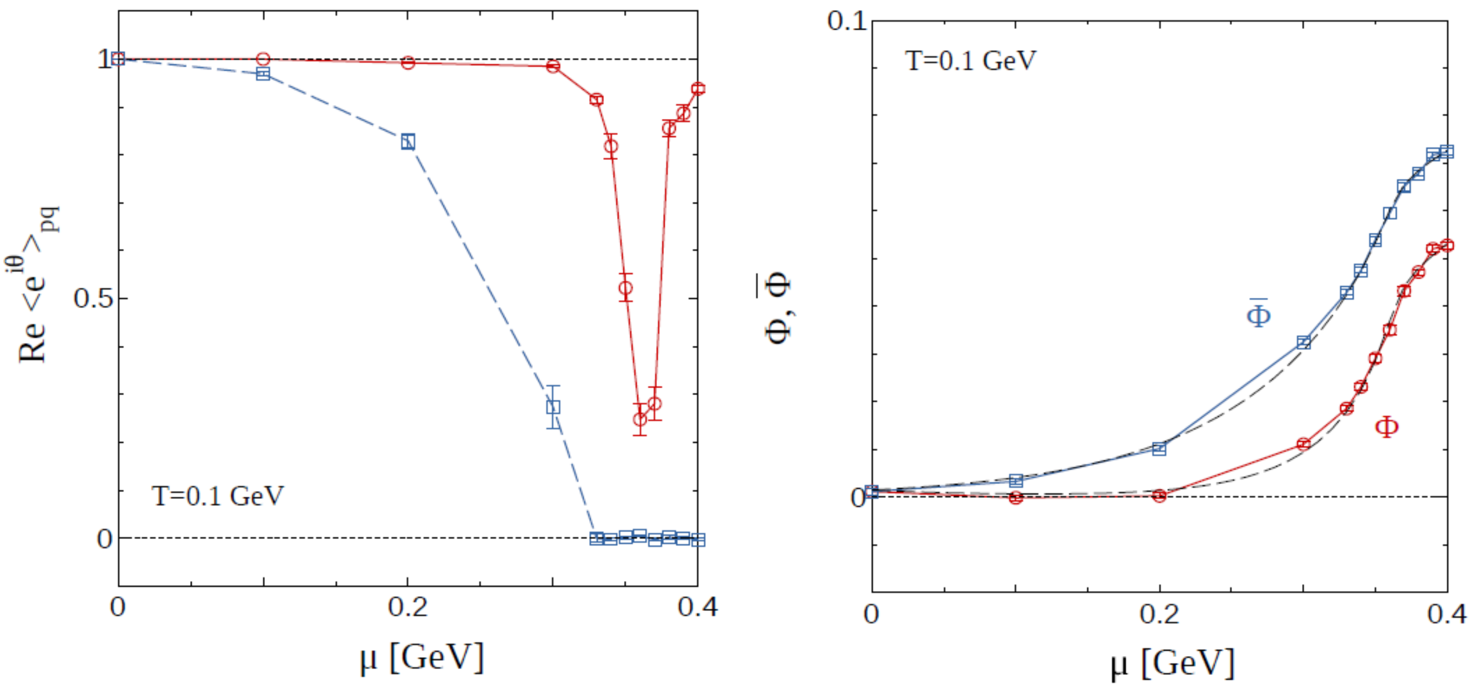




K. Kashiwa, Y. Mori, AO, PRD 99 ('19)

POM for PNJL with vector coupling

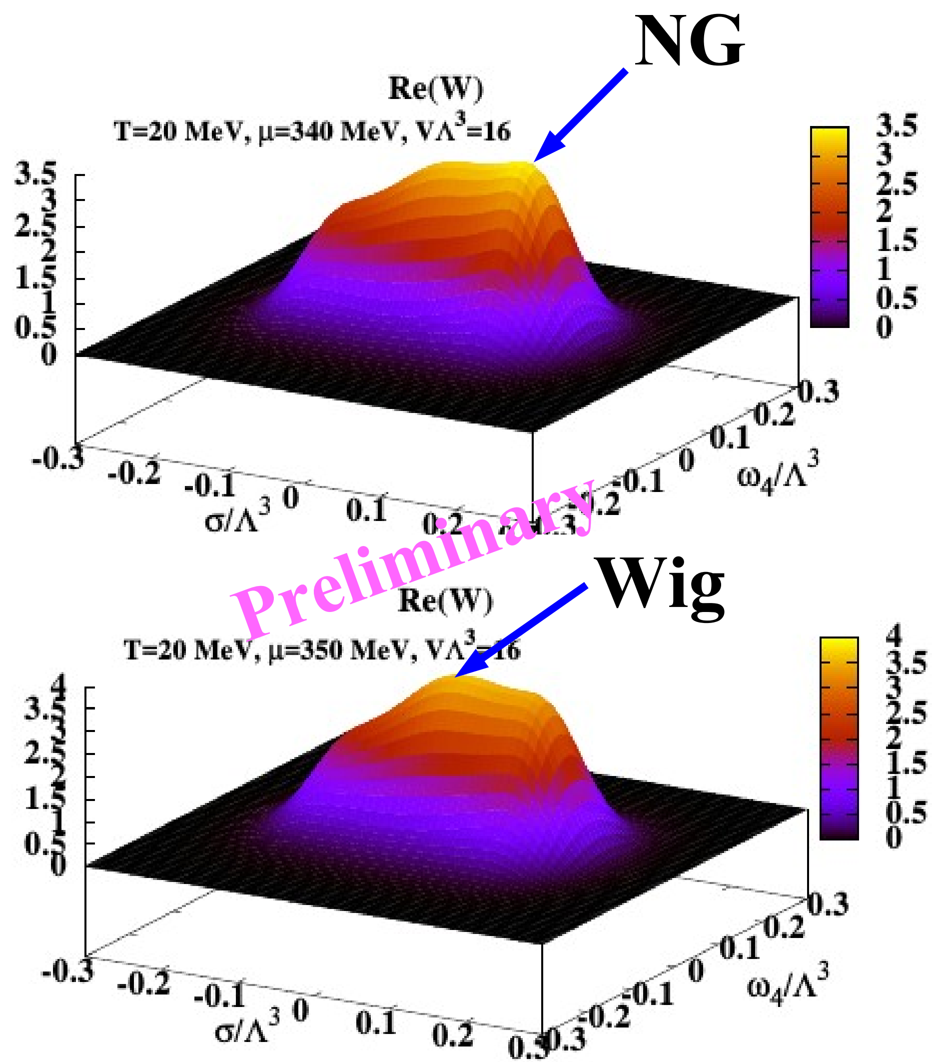
- **POM works in PNJLv**
  - **Pol. loop converges to MF results.**
  - **Average phase factor is enhanced significantly, but we still find the region, APF < 1 and we need special care for the initial config. distribution. (Optimization is not automatic in this case.)**



K. Kashiwa, Y. Mori, AO, arXiv:1903.03679

Do we describe multi thimbles ?

- **It seems yes.**
- **Statistical weight in NJLv on (σ, ω_4) plain after optimization on the 2D mesh.**
  → Three peaks (or shoulders)
- **Transition from the Nambu-Goldstone phase to the Wigner phase occurs at μ=(340-350) MeV**
- **In the V → ∞ limit, this corresponds to the phase transition. (We may need exchange MC or different tempering.)**

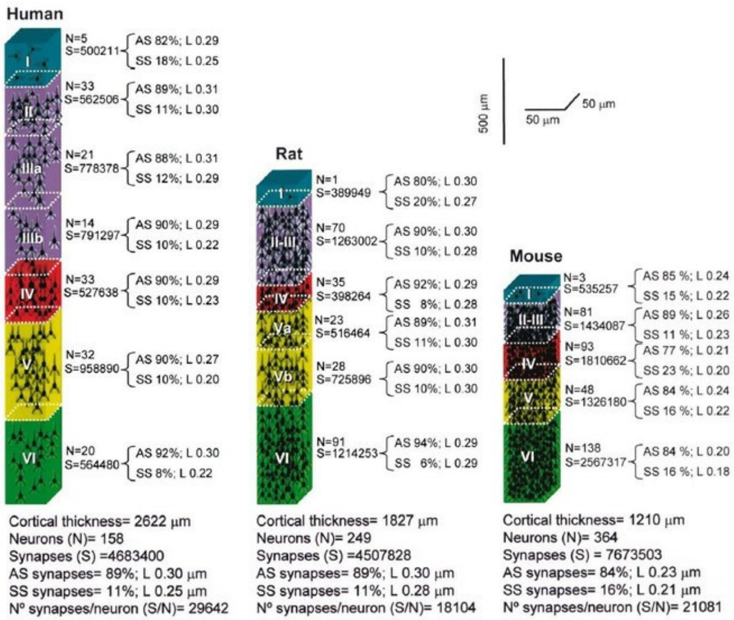


Summary

- Complexified variable methods (LTM, CLM, POM) are promising tools to tackle the sign problem. [c.f. Talk by Fukuma]
- Path optimization method has been demonstrated to work in
  1 dim. integral, 1+1 dim. scalar theory at finite density,
  0+1 dim. QCD, and PNJL model w/ and w/o vector coupling.
  - POM does not suffer from zero point of fermion det., since it is not a singular point of the Boltzmann weight.
  - Complex phase from Jacobian and the Boltzmann weight cancels with each other, and the residual sign problem is evaded.
  - In 1 dim. QCD, an apparent multimodal problem in the diag. gauge can be avoided by calc. w/o diag. gauge fixing.
  - Sometimes, the average phase factor does not easily grow during the optimization. Improving the opt. method and/or knowledge of preferred path would be necessary (not yet *ab initio*).
- To do: 1+1 D QCD, Reducing cost $O(V^3)$, ...

Prospect

- **Path optimization in 3+1 D field theories would require reduction of numerical cost.**
  Imaginary part
  = f (real parts of same point and nearest neighbor points)
  may be a good guess.
- **Deep learning (# of hidden layers > 3) may be helpful to explore complex paths, which human beings (~ 7 layers) cannot imagine, while "Understanding" the results of machine learning need to be done by human beings (at present).**



Defelipe 2011a (Review). The evolution of the brain, the human nature of cortical circuits, and intellectual creativity. Front Neuroanat 5, 29.

Thank you for your attention !

Fermion Determinant

Faldt, Petersson, 1986

- **Fermion action is separated to each spatial point and bi-linear → Determinant of Nτ x Nc matrix**

$$\exp\square V_{\rm eff}/T\square \int dU_0 \begin{vmatrix} I_1 & e^{\square} & 0 & & e^{-\square}U^{\square} \\ -e^{-\square} & I_2 & e^{\square} & & \\ 0 & -e^{-\square} & I_3 & e^{\square} & \\ \vdots & & & \ddots & \\ -e^{\square}U & & & -e^{-\square} & I_N \end{vmatrix}$$

Nc x Nτ

$$= \int dU_0 \det\left[X_N[\square]\otimes 1_c \square e^{-\square/T}U^{\square}\square\square 1\square^{N}\square e^{\square/T}U\right]$$

Nc

$$= X_N^3 - 2X_N\square 2\cosh\square 3N_{\square}\square$$

$$I_{\square}/2 = [\square\square x\ \square\square i\ \square\square x\ \square\square\square x\ \square]/2N_c\square^2\square m_0/\square$$

$$X_N = B_N\square B_{N-2}\square\ ;\ N-1\square$$

$$B_N = I_N B_{N-1}\square B_{N-2}$$

$$B_N = \begin{vmatrix} I_1 & e^{\square} & 0 & & \\ -e^{-\square} & I_2 & e^{\square} & & \\ 0 & -e^{-\square} & I_3 & e^{\square} & \\ \vdots & & & \ddots & \\ & & & -e^{-\square} & I_N \end{vmatrix}$$

Discussions

Frequently Asked Questions

- **How many parameters do you have ?**
  → Many ;) For generic trial funciton (V= # of variables)

$$y_i = y_i(x_1, x_2, \dots x_V)$$

$$N_{\mathrm{par}} = (N_{\mathrm{layer}} + 1) \times V \times (N_{\mathrm{unit}} + 1) + 2V$$

- **How about the numerical cost ?**
  → A lot ;) Derivative of J with respect to parameters cost most.

$$\frac{\partial J}{\partial c_i} = J \frac{\partial J^{-1}_{jk}}{\partial z_l} \frac{\partial z_l}{\partial c_i} \to \mathcal{O}(V^3)$$

- **It is still polynomial.**
  Does the sign problem becomes "P" problem?
  → No. The average phase factor is still exp(-# V).
  If extrapolation is possible from finite V, we have a hope.

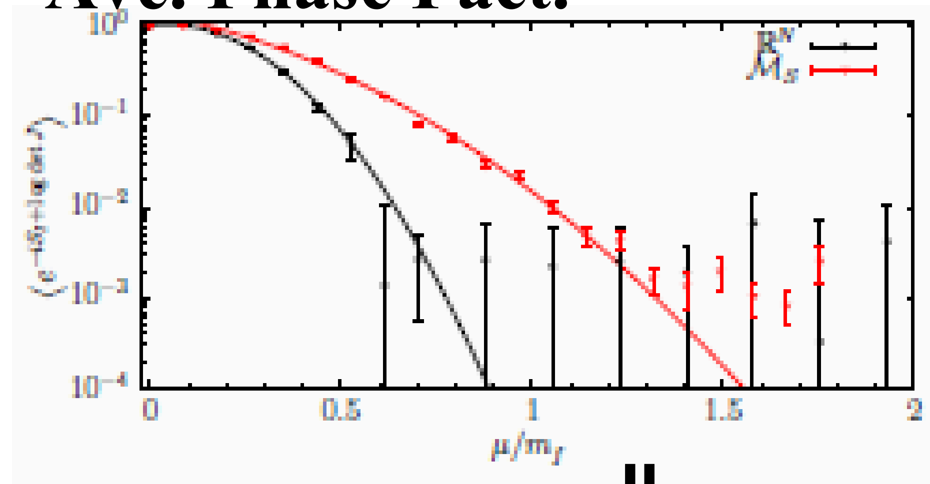
- **How can we reduce the cost ? → Next page**

How can we reduce the numerical cost ?

- **Restrict the function form of y(x).**
  - **Imaginary part is a function of its real part.**
    E.g. Alexandru, Bedaque, Lamm, Lawrence, PRD97('18)094510
    [Lawrence, Warrington, Lamm (Mon)]
    Thirring model, 1+1D QED

$$y_i = f(x_i), f(x) = \lambda_0 + \lambda_1 \cos x$$

Ave. Phase Fact.

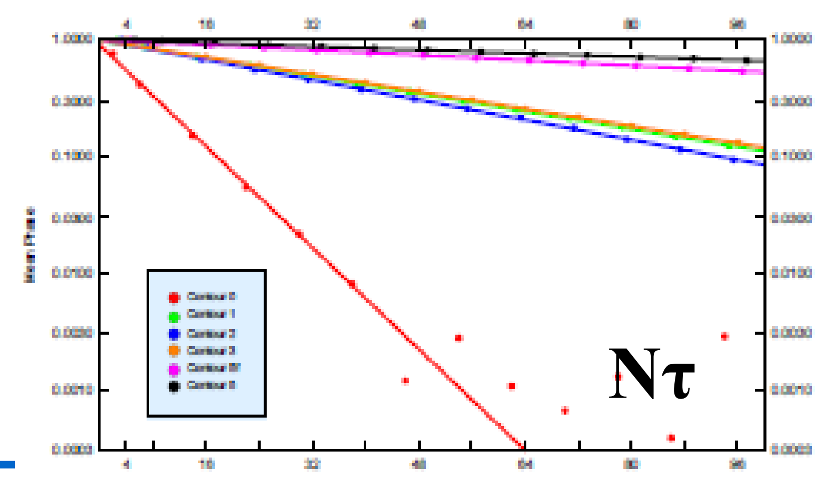


μ

  - **Nearest neighbor site**
    F. Bursa, M. Kroyter, arXiv:1805.04941
    0+1 D φ^4 theory
    Translational inv. + U(1) sym.

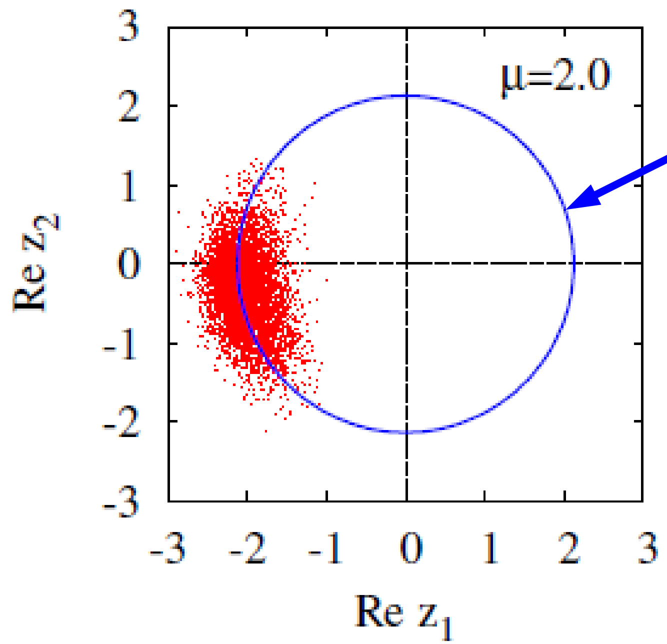
$$y_{a,i} = \frac{\varepsilon_{ab} x_{a,i+1}}{1 + x_{1,i}^2 + x_{2,i}^2}$$

Ave. Phase Fact.



Frequently Asked Questions (cont.)

- **What happens when we have 10^{10} fixed points ?**
→ In that case we should give up. (My answer @ Lattice 2017)
→ If those fixed points are connected by the symmetry,
we may be able to perform path optimization.

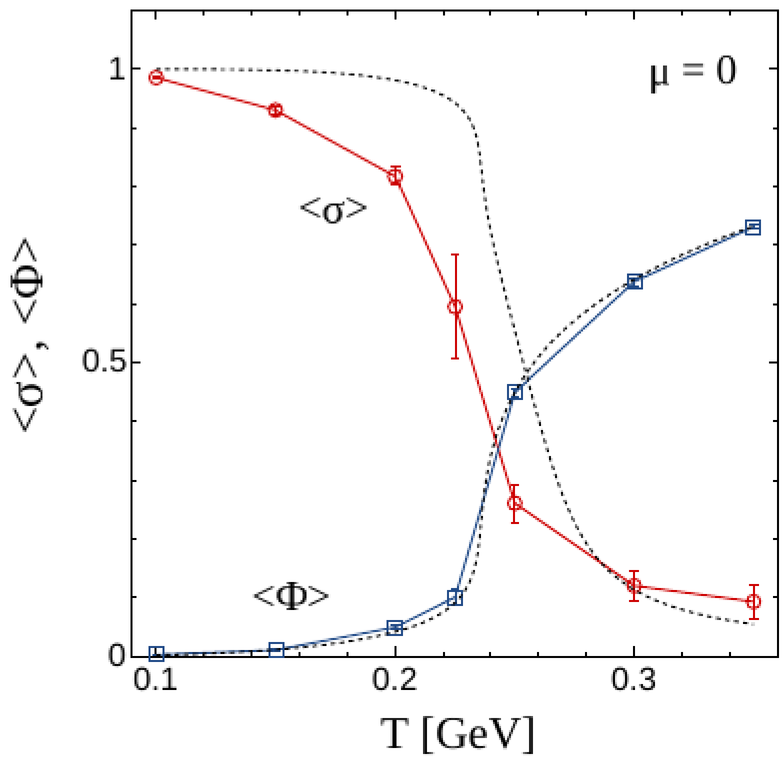


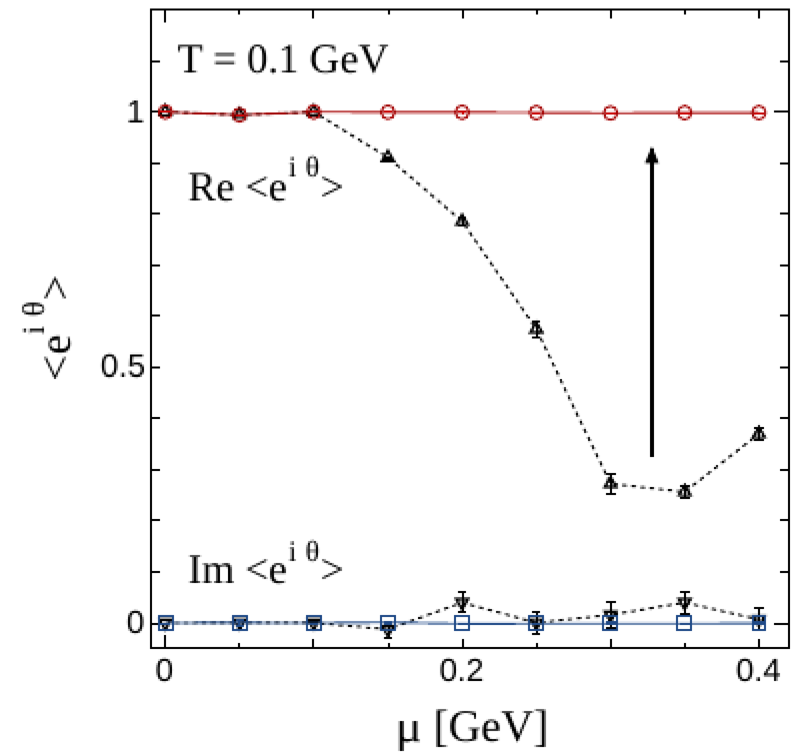
Mean field results
= Degenerate fixed points
(All have the same θ.)

If they have different complex phases, the global sign problem emerges and the partition function would be almost zero.
E.g. H. Fujii, S. Kamata, Y. Kikukawa, arXiv:1710.08524

Application to PNJL

- **PNJL model with homogeneous condensates, (σ, π, Φ, $\overline{\Phi}$).**
  - **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

- The sign problem is a grand challenge in theoretical physics, and appears in many fields of physics,
  - finite density QCD, real time evolution, Hubbard model off half-filling, other quantum MC with fermions, …

  and complexified variable methods (LTM, CLM, POM) would be promising to evade the sign problem.
- Path optimization with the use of the neural network is demonstrated to work in field theories having many variables.
  - 1+1D φ^4 theory at finite μ (neural network)
  - 0+1D QCD w/ fermions (grad. descent, neural network)
  - 3+1D homogeneous PNJL (neural network)
- Neural network (single hidden layer) is the simplest device of machine learning, and it helps us to generate and optimize generic multi-variable functions, $y_i=y_i(\{x\})$.

Prospect

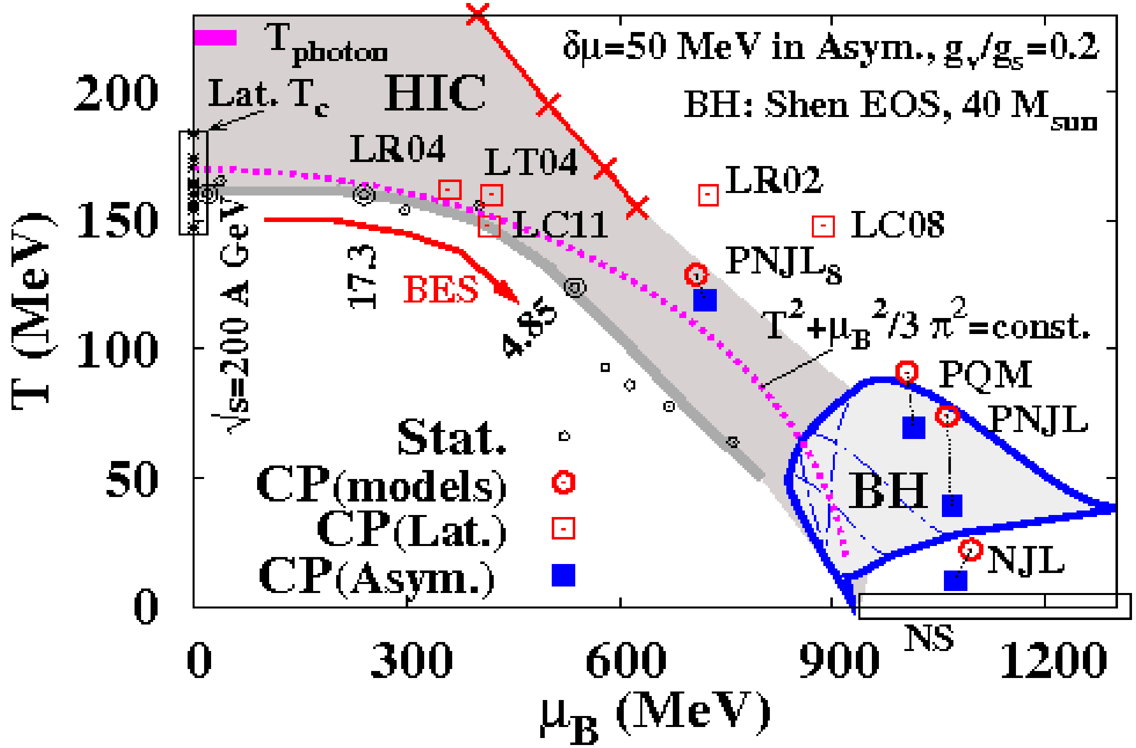
- **Path optimization in 3+1 D field theories would require reduction of numerical cost.**
  Imaginary part
  = f (real parts of same point and nearest neighbor points)
  may be a good guess.
- **Deep learning (# of hidden layers > 3) may be helpful to explore complex path, which human beings (~ 7 layers) cannot imagine, while "Understanding" the results of machine learning need to be done by human beings (at present).**

Thank you for your attention !

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 LQCD, …

AO, PTPS193('12)1.

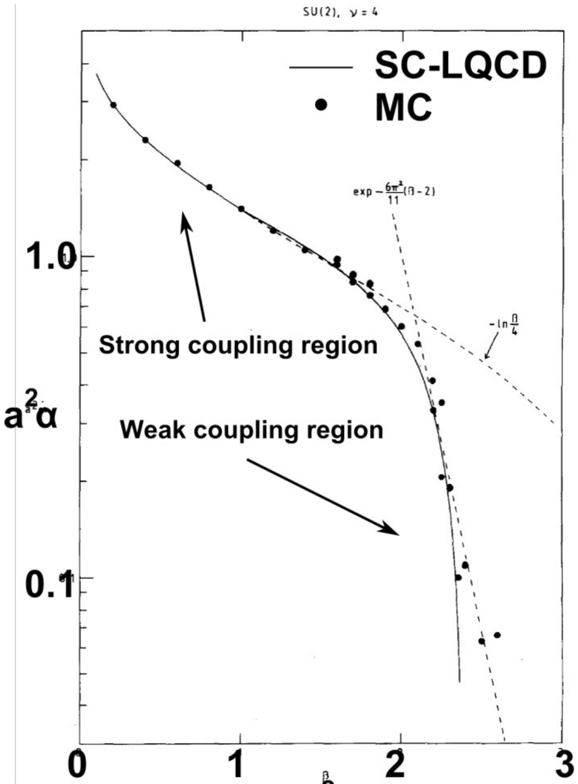


- Complex Langevin method (CLM)
  Parisi ('83), Klauder ('83), Aarts et al. ('11), Nagata et al. ('16)
- Lefschetz thimble method (LTM)
  E. Witten ('10), Cristoforetti et al. ('12), Fujii et al. ('13)
- Generalized LTM (GLTM)
  A. Alexandru, et al., ('16)

Complexified variable methods

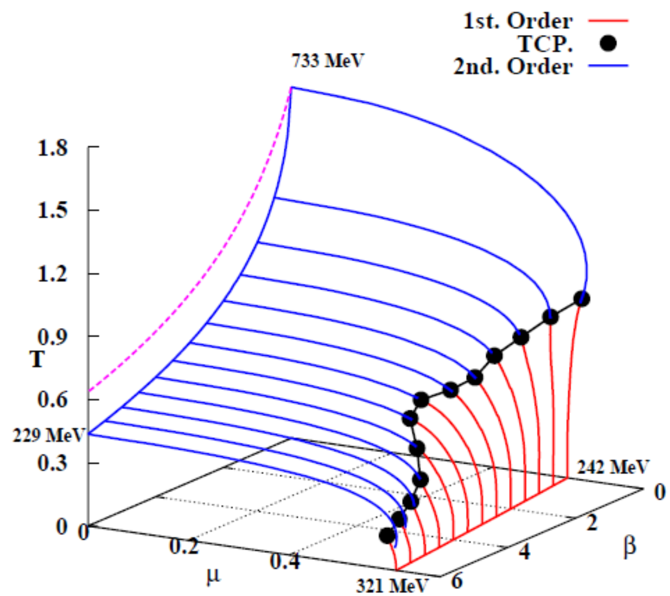
Strong Coupling Lattice QCD

Pure YM → Area Law



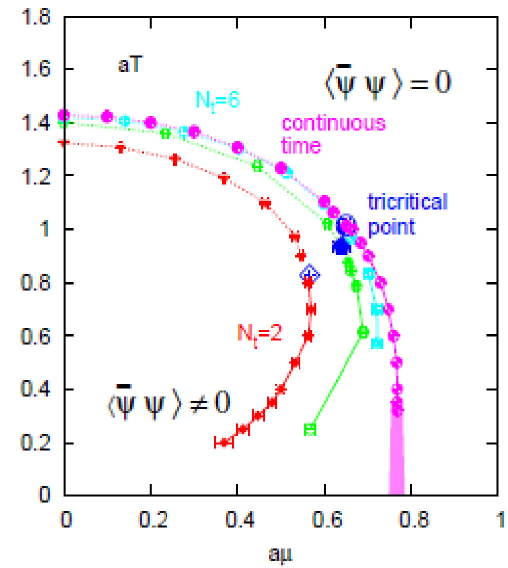
Wilson ('74), Creutz ('80), Munster ('80, '81), Lottini, Philipsen, Langelage's ('11)

Phase diagram (mean field)



Kawamoto ('80), Kawamoto, Smit ('81), Damagaard, Hochberg, Kawamoto ('85), Ilgenfritz, Kripfganz ('85), Bilic, Karsch, Redlich ('92), Fukushima ('03); Nishida ('03), Kawamoto, Miura, AO, Ohnuma ('07). Miura, Nakano, AO, Kawamoto ('09), Nakano, Miura, AO ('10), Miura, Kawamoto, Nakano, AO ('17)

Lattic MC simulations (Fluctuations)



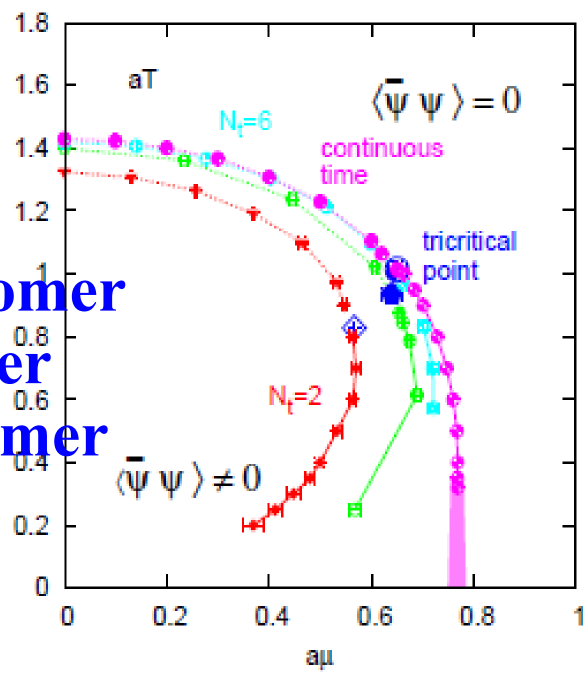
Rossi, Wolff ('84), Mutter, Karsch ('89), de Forcrand, Fromm ('10), de Forcrand, Unger ('11), AO, Ichihara, Nakano ('12), Ichihara, Nakano, AO ('14), de Forcrand, Langelage, Philipsen, Unger ('14), Ichihara, Morita, AO ('15)

Phase Diagram in Strong Coupling Lattice QCD

Aoki ('84), Rossi, Wolff ('84), Damagaard, Hochberg, Kawamoto ('85), Mutter, Karsch ('89), Bilic, Karsch, Redlich ('92), Fukushima ('03), Nishida ('03), Kawamoto, Miura, AO, Ohnuma ('07), Miura, Nakano, AO, Kawamoto ('09), Nakano, Miura, AO ('10), de Forcrand, Fromm ('10), de Forcrand, Unger ('11), Misumi, Nakano, Kimura, AO('12), Misumi, Kimura, AO('12), AO, Ichihara, Nakano ('12), Tomboulis ('13), Ichihara, Nakano, AO ('14), Ichihara, Morita, AO ('15)

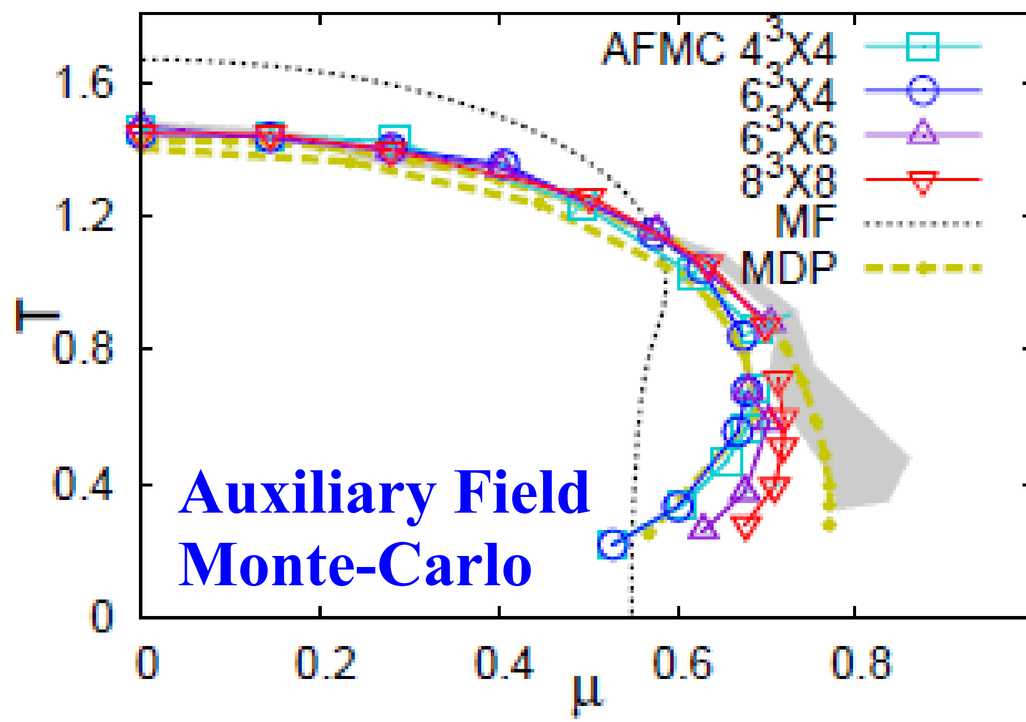
- **Integrate links first, and fermions later → Milder sign prob.**
- **Two indep. methods give consistent phase diagram in the *Strong Coupling Limit*.**

Monomer -Dimer -Polymer



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

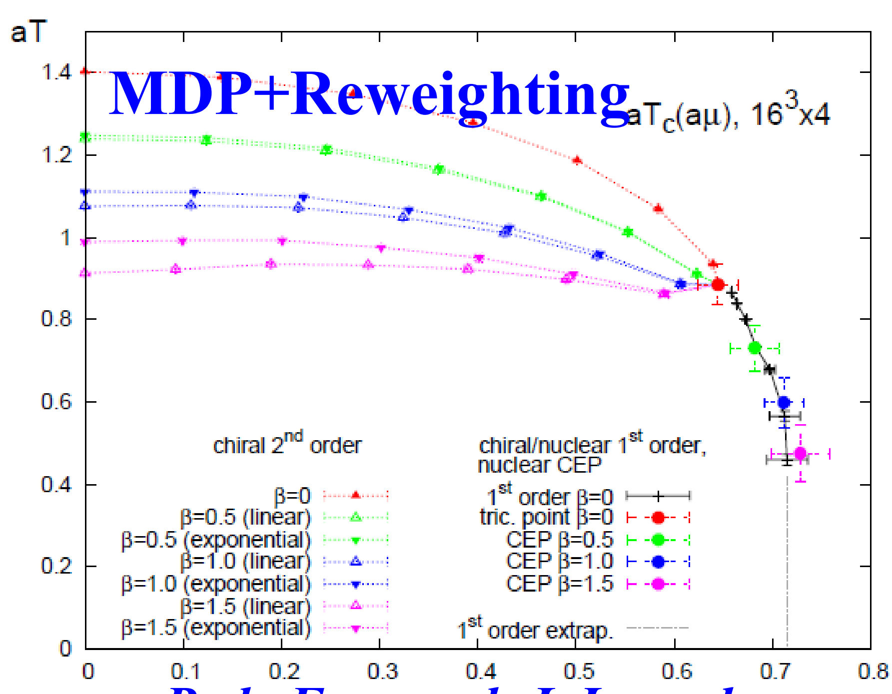
Auxiliary Field Monte-Carlo



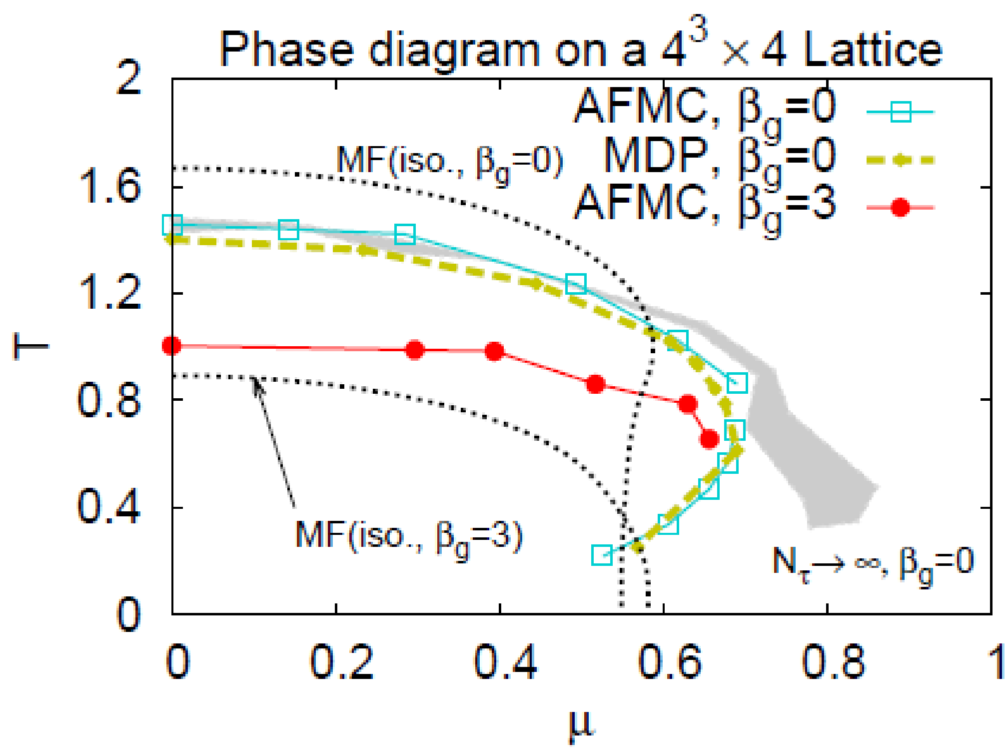
T.Ichihara, AO, T.Z.Nakano, PTEP2014,123D02.

Phase Diagram Away from the Strong Coupling Limit

- **Sampling at finite coupling ($g < \infty$ or $2N_c/g^2 > 0$) is difficult !**
  - **Monomer-Dimer-Polymer sim. → Reweighting from SCL**
    P. de Forcrand, J. Langelage, O. Philipsen, W. Unger ('14)
  - **Auxiliary Field Monte-Carlo**
    → Direct sampling is possible at small μ/T, but fails at large μ
    AO, T. Ichihara (Lattice 2015)



P. de Forcrand, J. Langelage, O. Philipsen, W. Unger ('14)



AO, Ichihara (Lattice2015)

Why is direct sampling difficult at finite $1/g^2$?
→ Sign problem from Repulsive Interaction

and also from the Polyakov loop ?
(U. Wenger on Mon.)

One of the origins of the sign problem = Repulsion

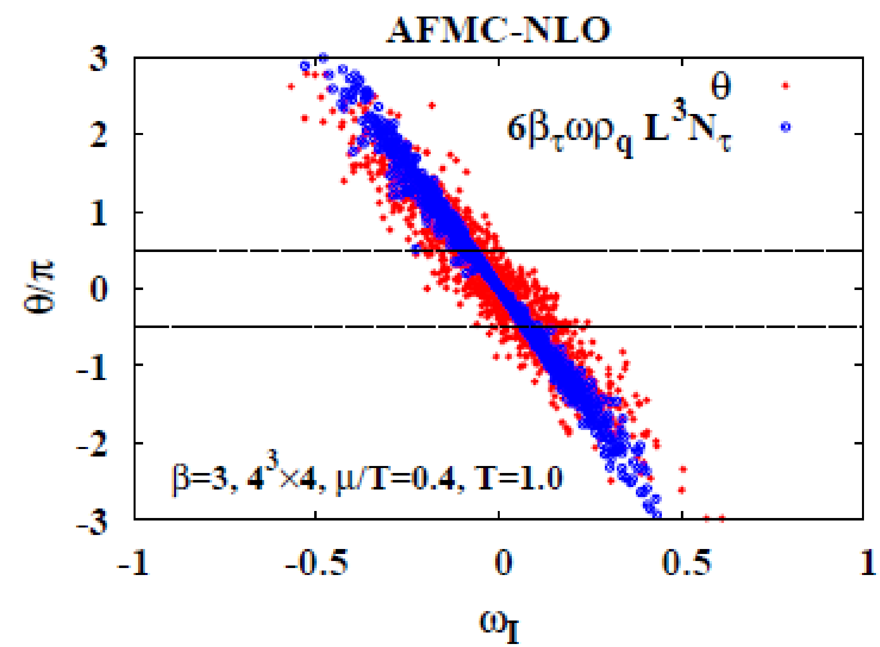
- **Repulsive 4-Fermi interaction → Sign prob. via Hubbard transf.**

$$\exp\left[-G^2(q^\dagger q)^2\right] = \int d\omega e^{-\omega^2/2 - iG(q^\dagger q)\omega}$$

- **With small fluctuation in density** $q^\dagger q \sim \rho$
  - **Phase ~ Gωρ x L³ → Serious sign prb.**

SIGN '18

International Workshop on the Sign Problem in QCD and Beyond



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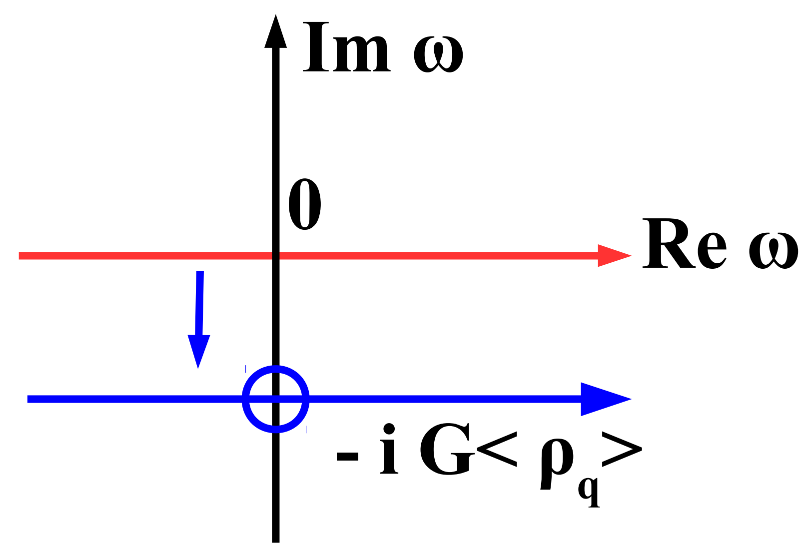
- **With small fluctuation in density** $q^\dagger q \sim \rho$
  - **Phase ~ Gωρ x L^3 → Serious sign prb.**
  - **Shifted ω should kill sign prb.**

$$-\frac{\omega^2}{2} - iG\omega\rho_q = -\frac{1}{2}(\omega + iG\rho_q)^2 - G^2\rho_q^2$$



Strong Coupling Lattice QCD action (1)

- **Lattice QCD action (unrooted staggered fermion)**

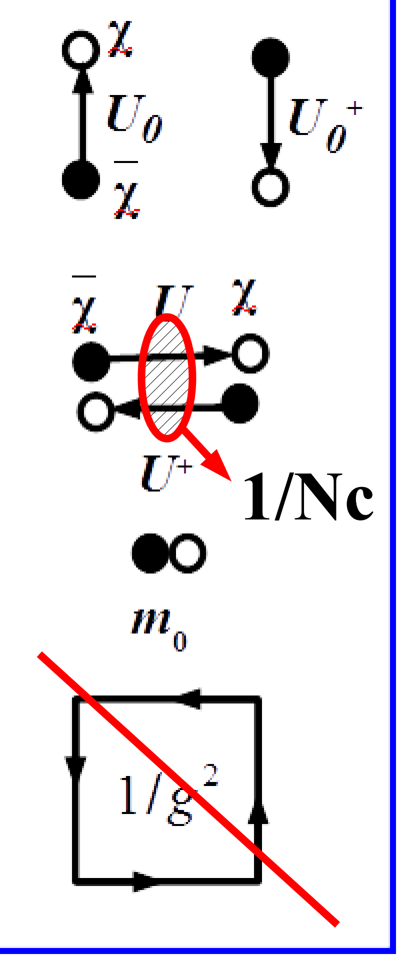
$$S = \frac{1}{2}\sum_{x,\mu}\left[\eta_\mu(x)\bar{\chi}_x U_\mu(x)\chi_{x+\hat{\mu}} - \eta_\mu^{-1}(x)\bar{\chi}_{x+\hat{\mu}}U_\mu^\dagger(x)\chi_x\right] + m_0\sum_x \bar{\chi}_x\chi_x$$
$$- \frac{2N_c}{g^2}\sum_P \mathrm{ReTr}U_P \quad \left(\eta_\nu(x) = (-1)^{x_0+\cdots+x_{\nu-1}}e^{\mu\delta_{\nu 0}}\right)$$

- **Eff. Action in the Strong Coupling Limit**
  Damgaard, Kawamoto, Shigemoto ('84),
  Jolicoeur, Kluberg-Stern, Lev, Morel, Petersson ('84).
  - **Spatial link integral→ Four-Fermi int. (LO in 1/d expansion)**

$$S_{\mathrm{eff}}^{(\mathrm{SCL})} = \frac{1}{2}\sum_x\left[V_x^+ - V_x^-\right] + m_0\sum_x M_x - \frac{1}{4N_c}\sum_{x,j}M_x M_{x+\hat{j}}$$

$$V_x^+ = \bar{\chi}_x e^{\mu}U_0(x)\chi_{x+\hat{0}},\ V_x^- = \bar{\chi}_{x+\hat{0}}e^{-\mu}U_0^\dagger(x)\chi_x,\ M_x = \bar{\chi}_x\chi_x$$

SCL → (Scalar-Pseudoscalar) 4-Fermi int.



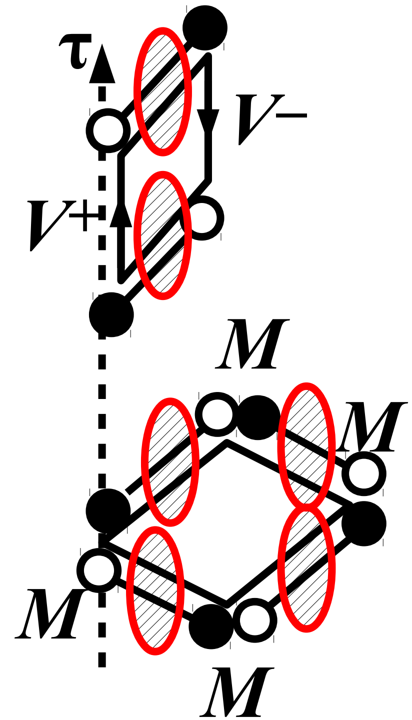
Strong Coupling Lattice QCD action (2)

- **$1/g^2$ correction**

Faldt, Petersson ('86), Miura, Nakano, AO, Kawamoto ('09)

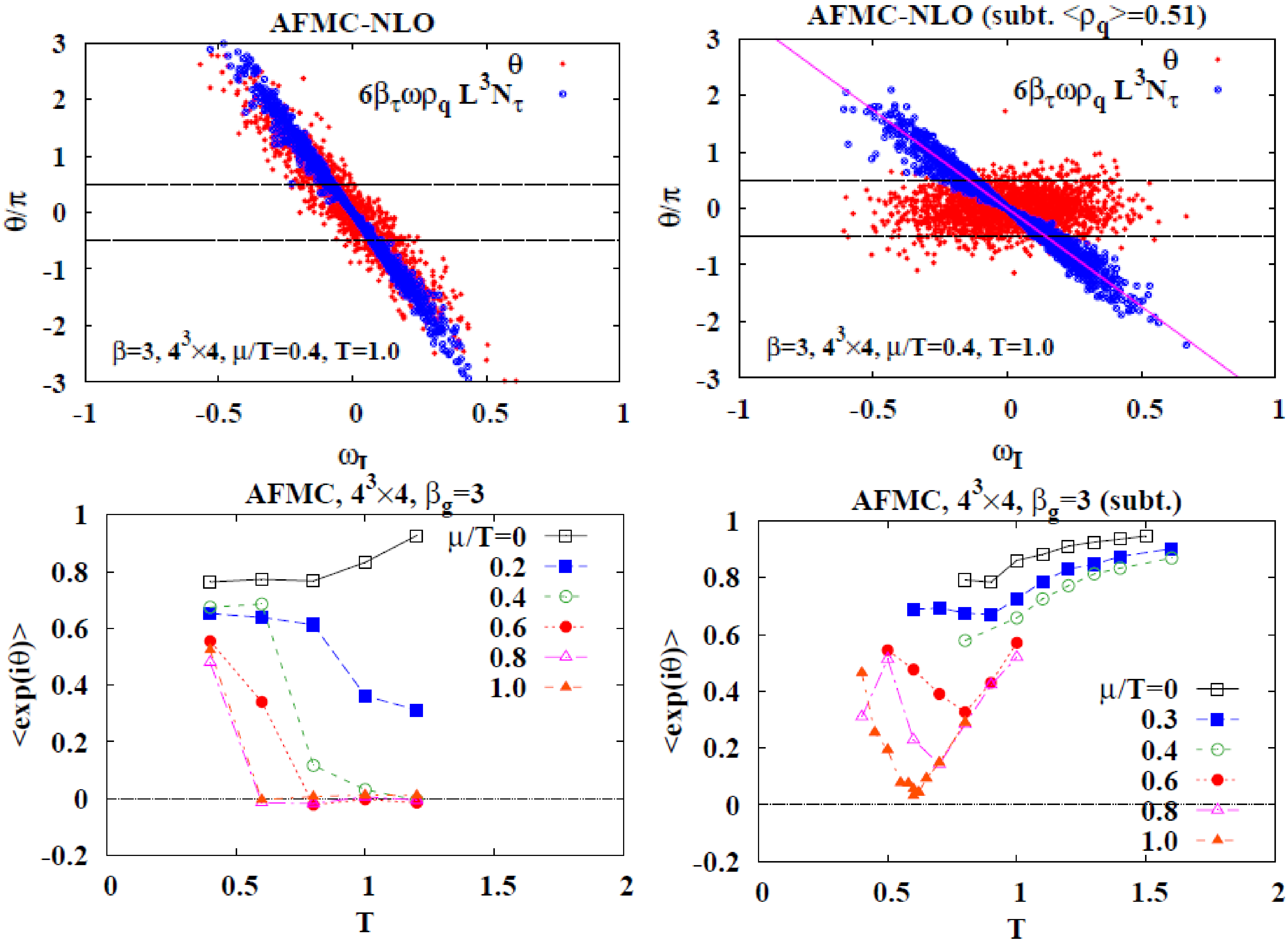
$$S_{\rm eff}^{\rm (NLO)} = S_{\rm eff}^{\rm (SCL)} + \frac{\beta_\tau}{2}\sum_{x,j}\left[V_x^+ V_{x+\hat{j}}^- + V_x^- V_{x+\hat{j}}^+\right] - \beta_s \sum_{x,k,j,k\neq j} M_x M_{x+\hat{j}} M_{x+\hat{j}+\hat{k}} M_{x+\hat{k}}$$

$$\beta_\tau = 1/2N_c^2 g^2,\ \beta_s = 1/16N_c^4 g^2$$



Plaquet ($1/g^2$) corr. generates
- *Density-Density (VV) 4-Fermi Repulsion*
- *8 Fermi attraction*

Imaginary Part Shifted AFMC works !



AO, Ichihara (Lattice2015)

When density fluctuation is small, auxiliary field shift of the imaginary part by constant works well.

However, when density fluctuation is large (e.g. around the 1st order phase transition), simple shift does not work.

Configuration dep. shift of the imaginary part → Complexified variable methods (LTM, CLM, GTM, POM, ...)

Contents

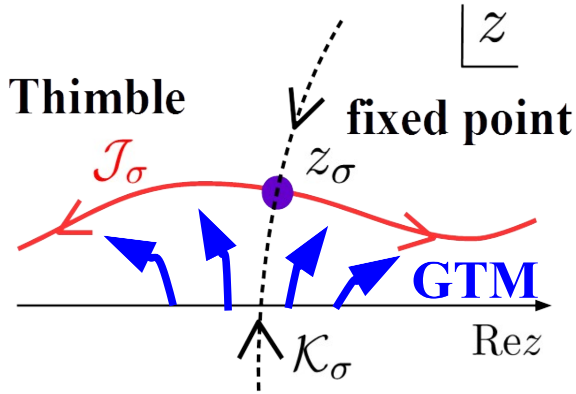
- **Introduction**
- **Path Optimization Method**
  Y. Mori, K. Kashiwa, AO, PRD 96 ('17), 111501(R) [arXiv:1705.05605]
  AO, Y. Mori, K. Kashiwa, EPJ Web Conf. 175 ('18), 07043 [arXiv:1712.01088] (Lattice 2017 proceedings)
- **Application to field theory using neural network**
  Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [arXiv:1709.03208]
- **Application to gauge theory: 1-dimensional QCD**
  → Talk by Yuto Mori (next talk)
- **Application to effective models with phase transition**
  K. Kashiwa, Y. Mori, AO, arXiv:1805.08940 and in prep.
- **Discussions**
- **Summary**

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)

Lefschetz thimble method

E. Witten ('10), Cristoforetti et al. (Aurora) ('12), Fujii et al. ('13), Alexandru et al. ('16). [Alexandru (Tue)]



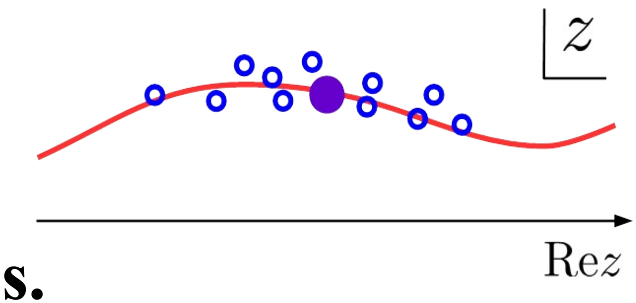
- **Solving the flow eq. from a fixed point σ**
  → Integration path (thimble)
  Note: Im(S) is constant on one thimble

$$\mathcal{J}_\sigma : \frac{dz_i(t)}{dt} = \overline{\left(\frac{\partial S}{\partial z_i}\right)} \to \frac{dS}{dt} = \sum_i \left|\frac{\partial S}{\partial z_i}\right|^2 \in \mathbb{R}, \quad \mathcal{C} = \sum_\sigma n_\sigma \mathcal{J}_\sigma$$

- **Problem:**
  - **Phase from the Jacobian (residual. sign pr.),**
  - **Different Phases of Multi-thimbles (global sign pr.),**
  - **Numerical Cost,**
  - **Stokes phenomena, …**

Complex Langevin method

Parisi ('83), Klauder ('83), Aarts et al. ('11),
Nagata et al. ('16); Seiler et al. ('13), Ito et al. ('16).
[Sexty (Mon), Stamatescu (Tue)]



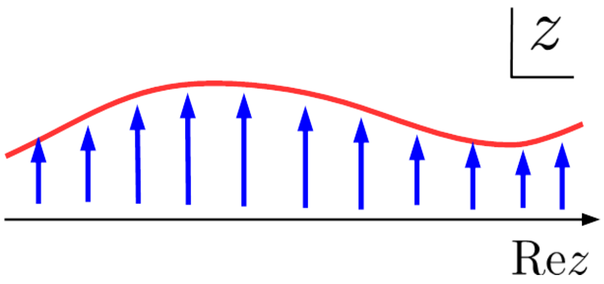
- **Solving the complex Langevin eq.→ Configs.**

$$\frac{dz_i}{dt} = -\frac{\partial S}{\partial z_i} + \eta_i(t) (\eta_i : \text{White noize}),\ \langle \mathcal{O}(x) \rangle = \langle \mathcal{O}(z) \rangle$$

- **No sign problem.**
- **Problem:**
  - **CLM can give converged but wrong results,**
    and we cannot know if it works or not in advance.

Path optimization method

Mori et al. ('17), AO, Mori, Kashiwa (Lattice 2017),
Mori et al. ('18), Kashiwa et al. ('18);
Alexandru et al. ('17 (Learnifold), '18 (SOMMe), '18),
Bursa, Kroyter ('18).
[Alexandru(Tue), Mori, Lawrence , Kroyter (Wed)]



- **Integration path is optimized to evade the sign problem, i.e. to enhance the average phase factor.**

$$\mathrm{APF} = \langle e^{i\theta} \rangle_{\mathrm{pq}} = \int dx e^{-S} \Big/ \int dx |e^{-S}| = \mathcal{Z}/\mathcal{Z}_{\mathrm{pq}}$$

Sign Problem → Optimization Problem

- **Cauchy(-Poincare) theorem: the partition fn. is invariant if**
  - **the Boltzmann weight W=exp(-S) is holomorphic (analytic),**
  - **and the path does not go across the poles and cuts of W.**
- **At Fermion det.=0, S is singular but W is not singular**
  - **Problem: quarter/square root of Fermion det.**

Cost Function and Optimization

- **Cost function: a measure of the seriousness of the sign problem.**

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

$$= |\mathcal{Z}| \left(\left| \langle e^{i\theta} \rangle_{\mathrm{pq}} \right|^{-1} - 1 \right) = \mathcal{Z}_{\mathrm{pq}} - |\mathcal{Z}|$$

$$\left[\theta = \arg(J e^{-S}),\ \theta_0 = \arg(\mathcal{Z}) \right]$$

- **Optimization: the integration path is optimized to minimize the Cost Function. (via Gradient Descent or Machine Learning)**
  - **Example: One-dim. integral → Complete set**

$$z(x) = x + iy(x),\ y(x) = \sum_n c_n H_n(x)$$

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

Benchmark test: 1 dim. integral

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

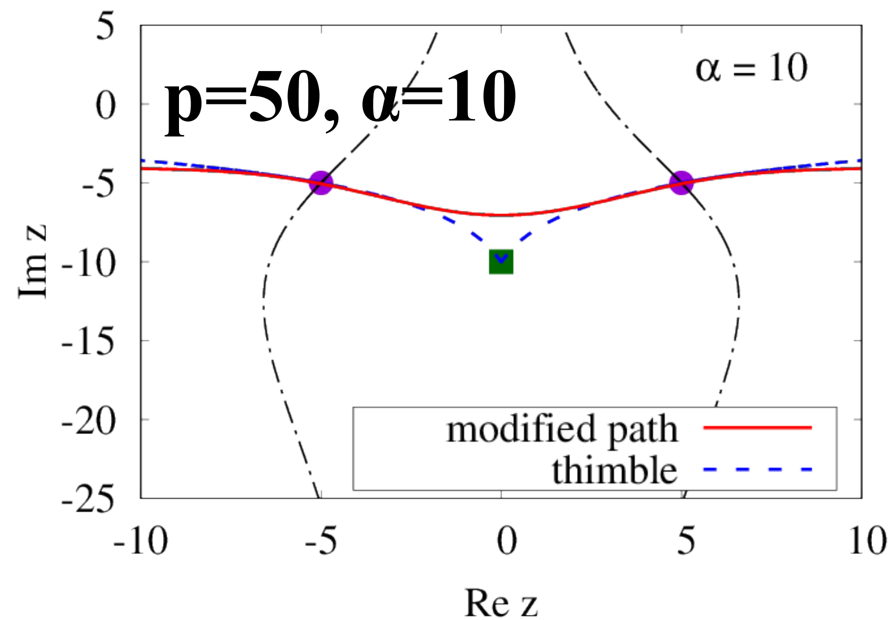
$$\mathcal{Z} = \int dx (x + i\alpha)^p \exp(-x^2/2)$$

  - **Sign prob. is serious with large *p* and small *α* → CLM fails**

- **Path optimization**

$$y(x) = c_1 \exp(-c_2^2 x^2/2) + c_3, \ \ J = 1 + i dy/dx$$

  - **Gradient Descent optimization**
  - **Optimized path ~ Thimble around Fixed Points**



Mori, Kashiwa, AO ('17); AO, Mori, Kashiwa (Lat 2017)

Benchmark test: 1 dim. integral

- **Stat. Weight J e^{-S}**

On Real Axis

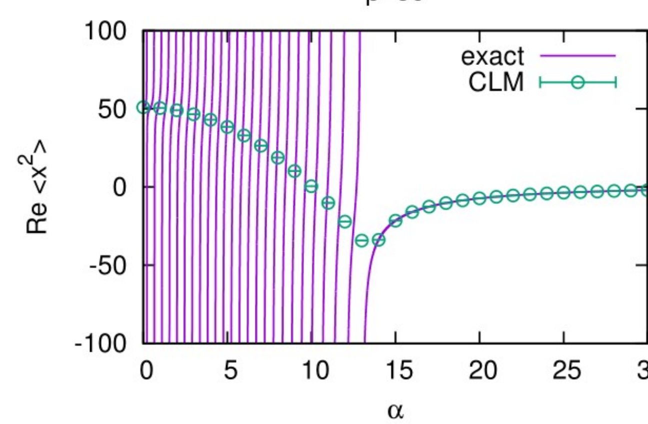
$(\times 10^{50})$

On Optimized Path

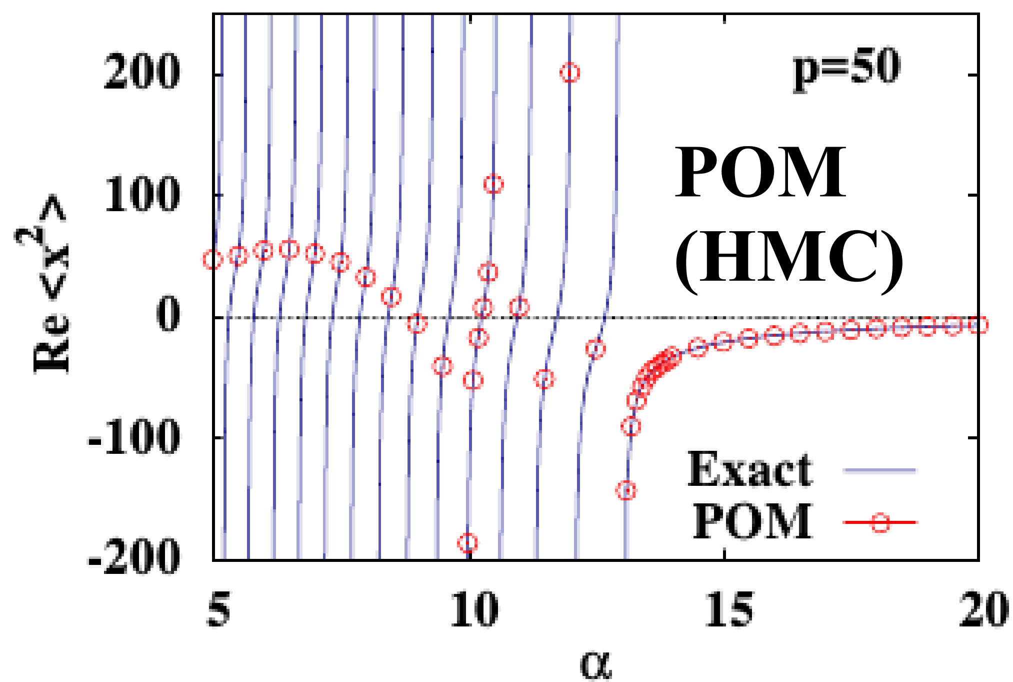
$(\times 10^{42})$

- **Observable**

CLM *Nishimura, Shimasaki ('15)*



vs



Mori, Kashiwa, AO ('17); AO, Mori, Kashiwa (Lat 2017)

Now it's the time to apply POM to field theories !

Application of POM to Field Theory

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

$$z_i(x) = x_i + i \sum_{n_1,n_2,\dots} c_i(n_1 n_2 \dots) H_{n_1}(x_1) H_{n_2}(x_2) H_{n_3}(x_3) \cdots$$

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

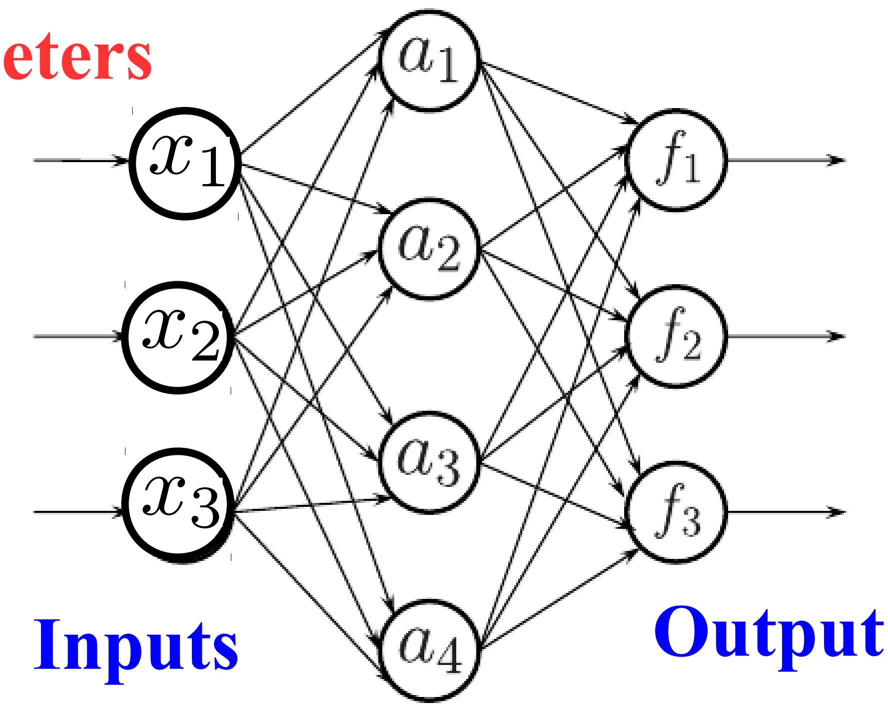
$$a_i = g(\underline{W_{ij}^{(1)}} x_j + \underline{b_i^{(1)}})$$

parameters

$$f_i = g(\underline{W_{ij}^{(2)}} a_j + \underline{b_i^{(2)}})$$

$$z_i = x_i + i(\underline{\alpha_i} f_i(x) + \underline{\beta_i})$$

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



  - **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

Grad. Desc. :

$dc_i/dt = -\partial\mathcal{F}/\partial c_i$

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

Hybrid Monte-Carlo with Neural Network

Initial Config. on Real Axis

HMC $H(x,p) = \frac{p^2}{2} + \mathrm{Re}S(z(x))$

Jacobian
→ via Metropolis judge

Do k = 1, N_epoch
Do j = 1, N_conf/N_batch

Mini-batch training of Neural Network

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

Grad. wrt parameters
(N_batch configs.)

$$F_i = \frac{1}{N_{\mathrm{batch}}} \sum_n \partial \mathcal{F}(n)/\partial c_i$$

Enddo

New N_conf configs. by HMC

$$H(x,p) = \frac{p^2}{2} + \mathrm{Re}S(z(x))$$

Enddo

N_batch ~ 10, N_conf ~ 10,000, N_epoch ~ (10-20)

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)

Comments in order

- **Neural Network in POM → Unsupervised Learning**
  - **We do not prepare "Teacher data" with problems and answers, but we prepare "Training data".**
  - **When APF increases, we can judge that "NN learned".**
    c.f. Learnifold: Machine learning of GTM manifold
    (Alexandru (Tue))
- **Sign problem ~ (almost) "NP hard" problem**
  - **Once the optimized path (answer) is given, we can examine the result (average phase factor) in MC simulations.**

Application to complex φ^4 theory using neural network

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

Complex φ⁴ theory at finite μ

- **Complex φ⁴ theory**

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

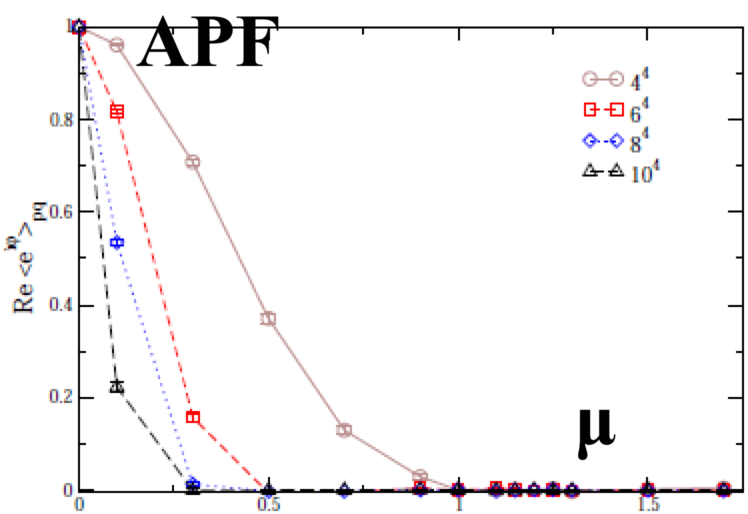
- **Action on Eucledean lattice at finite μ.**

$$S = \sum_x \left[\frac{(4+m^2)}{2} \phi_{a,x}\phi_{a,x} + \frac{\lambda}{4}(\phi_{a,x}\phi_{a,x})^2 - \phi_{a,x}\phi_{a,x+\hat{1}} - \cosh\mu\, \phi_{a,x}\phi_{a,x+\hat{0}} \right.$$

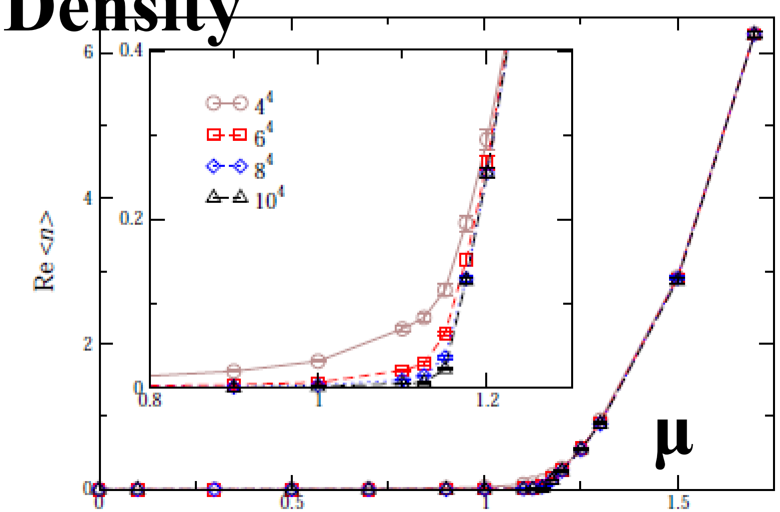
$$\left. \underline{+i\epsilon_{ab}\sinh\mu\, \phi_{a,x}\phi_{b,x+\hat{0}}} \right] \quad \left(\phi = \frac{1}{\sqrt{2}}(\underline{\phi_1} + i\underline{\phi_2}) \right)$$

complex **Complexify**

APF



Density



Complex Langevin & Lefschetz thimble work.

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

POM result (1): Average phase factor

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

APF

APF

μ

Optimization

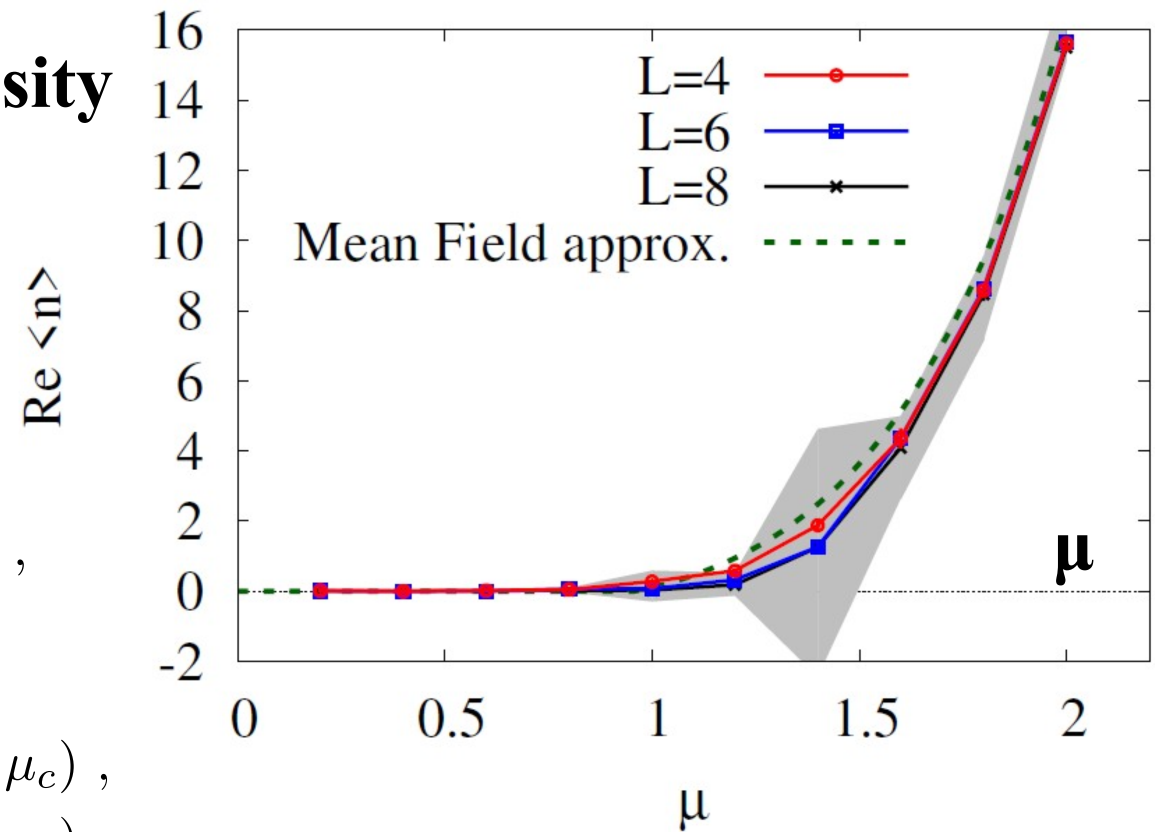
μ

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

Density



Mean Field App.

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

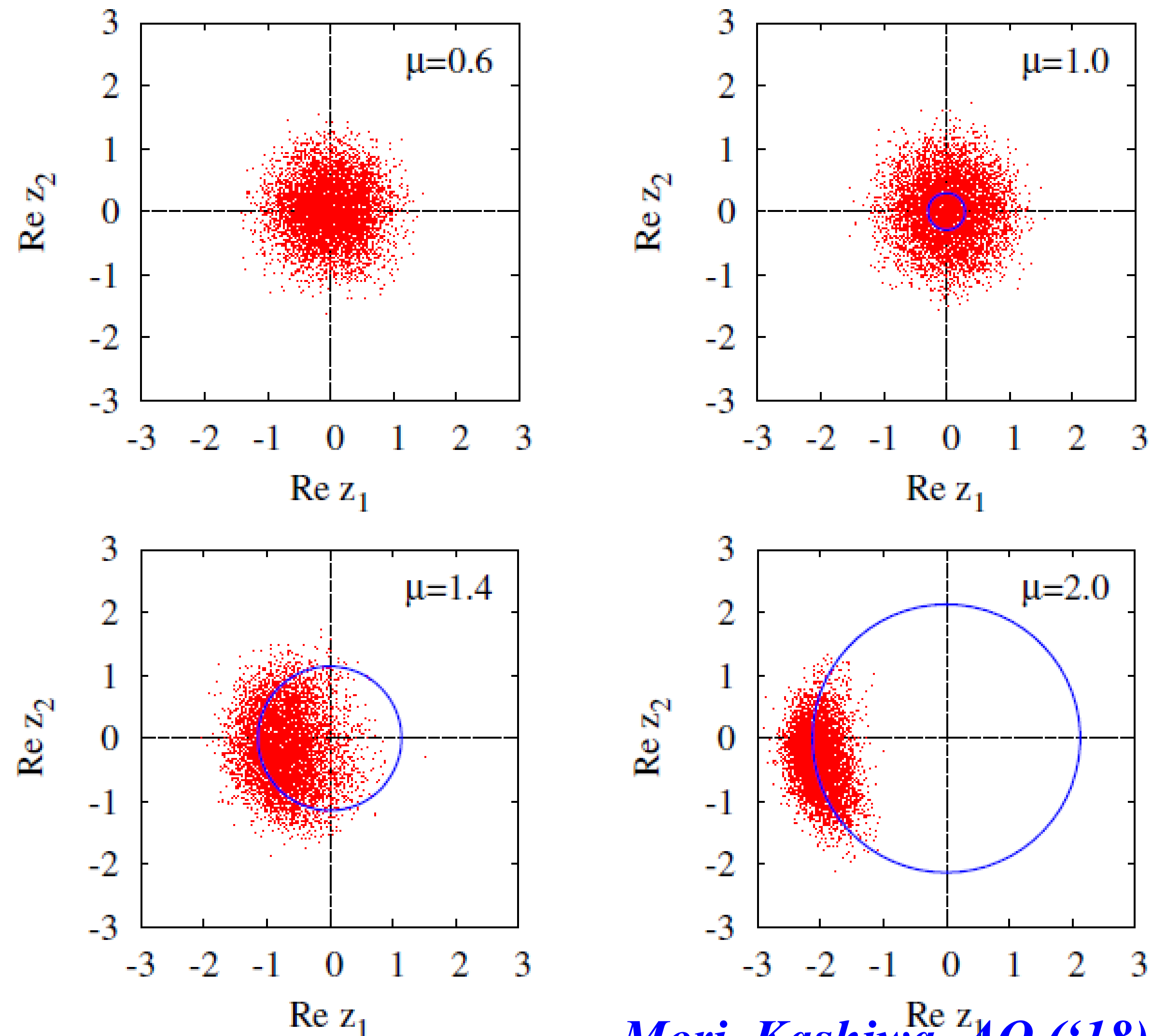
$$n = \phi^2 \sinh\mu \ ,$$

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

Mori, Kashiwa, AO ('18)

POM result (3): Configurations

- **Updated configurations after optimization**
  → sampled around the mean field results
- **Global U(1) symmetry in (φ_1, φ_2) is broken(*) by the optimization or by the sampling.**



*** This does not contradict the Elitzur's theorem.**

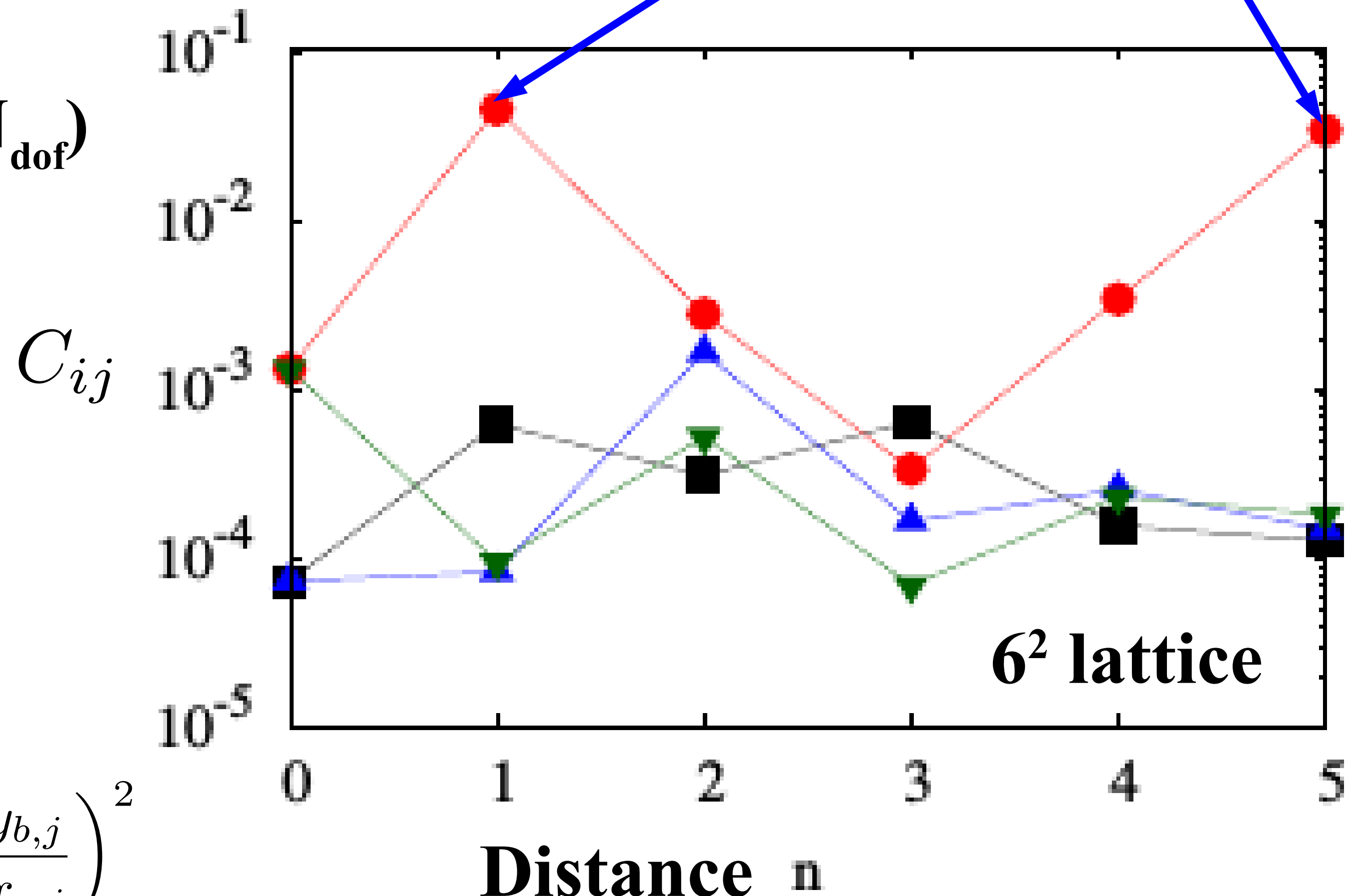
Mori, Kashiwa, AO ('18)

Which y's should be optimized ?

- Correlation btw (z_1,z_2) of temporal nearest neighbor sites are strong. Other correlations ~ 10^{-2} times smaller

$$\mathrm{Im}(S) = \sum_x \epsilon_{ab} \sinh \mu\, \phi_{a,x} \phi_{b,x+\hat{0}}$$

- Hope to reduce the cost to be $O(N_{dof})$



$$C_{ij} \equiv \left(\frac{\partial y_{a,i}}{\partial x_{b,j}}\right)^2 + \left(\frac{\partial y_{b,j}}{\partial x_{a,i}}\right)^2$$

Y. Mori, Master thesis

Application to Gauge Theory: 1 dimensional QCD

⇨ **Next Talk (by Yuto Mori)**

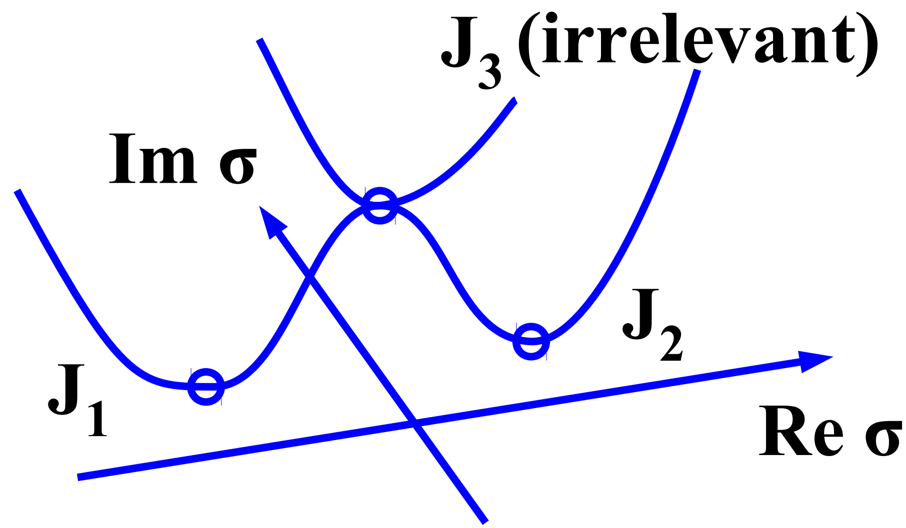
Y. Mori, K Kashiwa, AO, in prep.

Application to Effective Models with Phase Transition

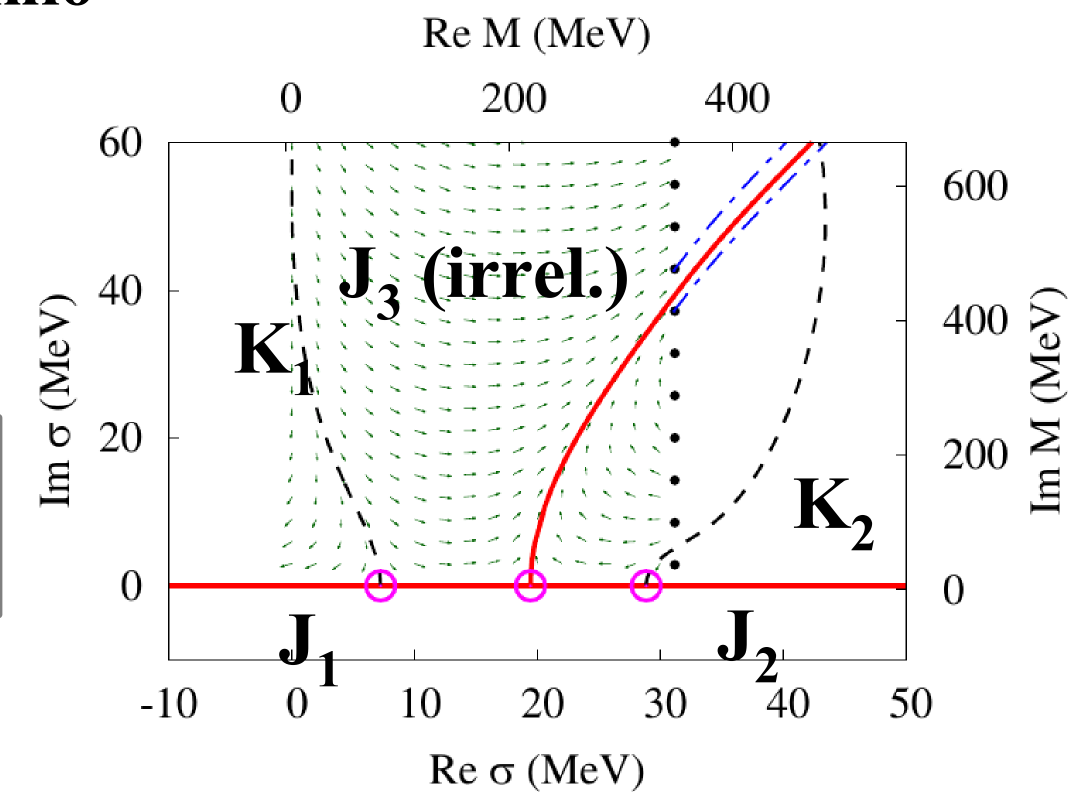
Y. Mori, K. Kashiwa, AO, PLB 781('18),698 [arXiv:1705.03646]
K. Kashiwa, Y. Mori, AO, arXiv:1805.08940 and in prep.

Complexified Variable Methods with Phase Transition

- **Phase transition**
  - **Transition of the dominant weight from a thimble to another thimble.**
  - **Thimble structure would be complicated.**



- **Thimbles in Nambu-Jona-Lasinio model** *Mori et al. ('18b)*
  - **Complicated structure with many cuts from log.**



Does POM work in Eff. models with P.T. ?

Y. Mori, K. Kashiwa, AO, PLB 781('18),698 [arXiv:1705.03646]

Application to PNJL

- **Polyakov-loop implemented NJL model with homogeneous auxiliary field anzats of (σ, π, Φ, $\overline{\Phi}$).**

$$\Gamma_{\rm PNJL} = \int d^4x \left[\bar{q}(-i \not{D} + m_0 - \mu\gamma_0)q - G\left\{(\bar{q}q)^2 + (\bar{q}i\vec{\tau}q)^2\right\}\right] + \frac{V}{T}\mathcal{V}_\Phi(\Phi,\bar{\Phi}) \simeq \frac{V}{T}\left[\mathcal{V}_{\rm NJL} + \mathcal{V}_\Phi\right]$$

Pol. loop pot.

$$\mathcal{V}_{\rm NJL} = -2N_f \int \frac{d^3p}{(2\pi)^3}\left[N_c \underline{E_p} - N_c\sqrt{\mathbf{p^2 + m_0^2}} + T\log(\underline{f^- f^+})\right] + G(\sigma^2 + \vec{\pi}^2)$$

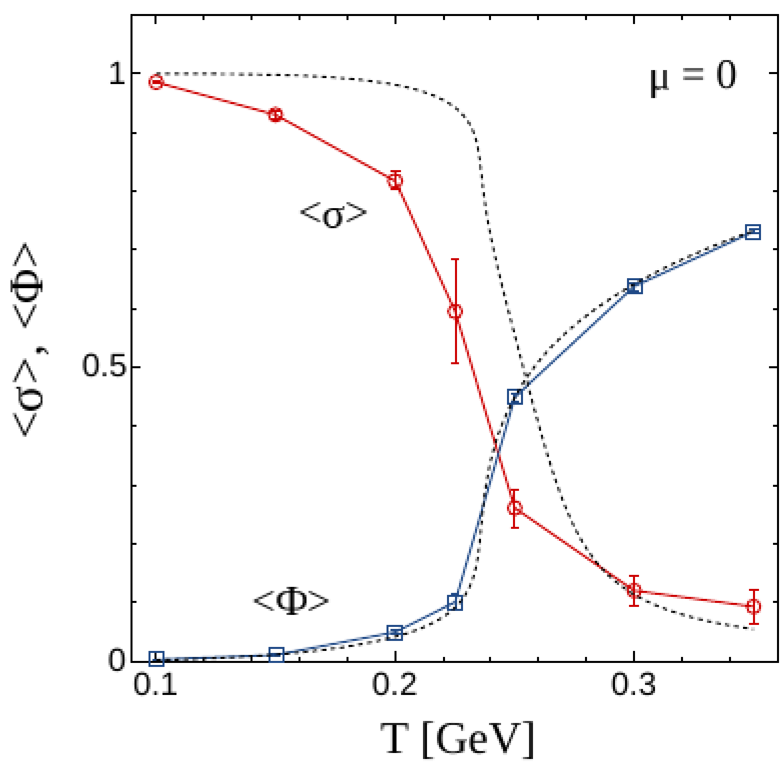
σ, π **σ, π, Φ, $\overline{\Phi}$**

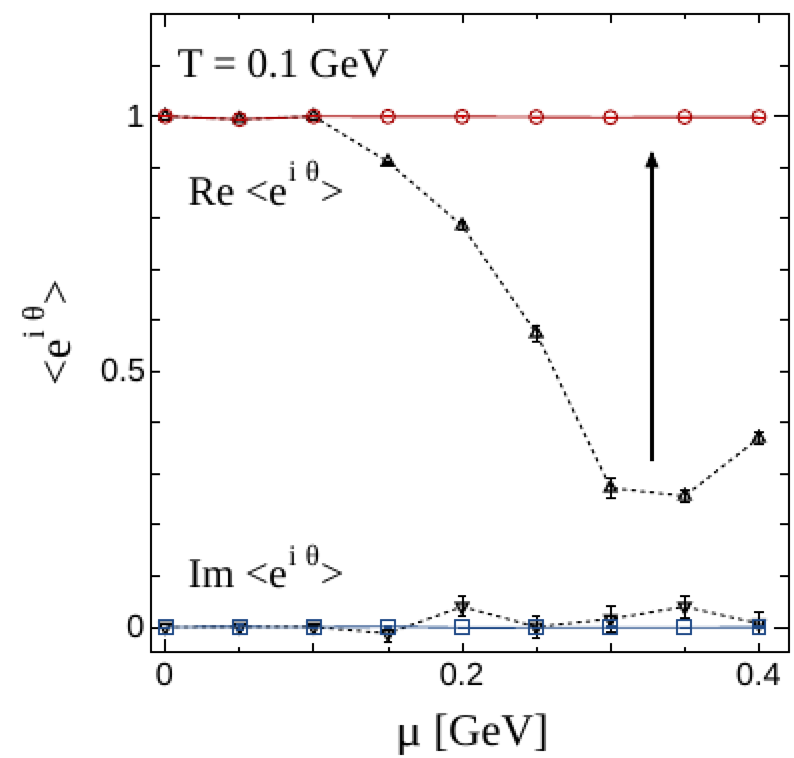
- **Action (Γ) has the imaginary part.**
- **The sign problem exists at finite volume. (Mean field becomes exact at infinite volume.)**

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

Application to PNJL

- **Path optimization for (A_3, A_8) with V=k/T^3, k=64.**
  - **Transition from Confined NG phase to Deconfined Wigner phase**
  - **Ave. Phase Factor ~ 0.25 around P.T. → ~ 1 after optimization**





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

PNJL with Vector Coupling

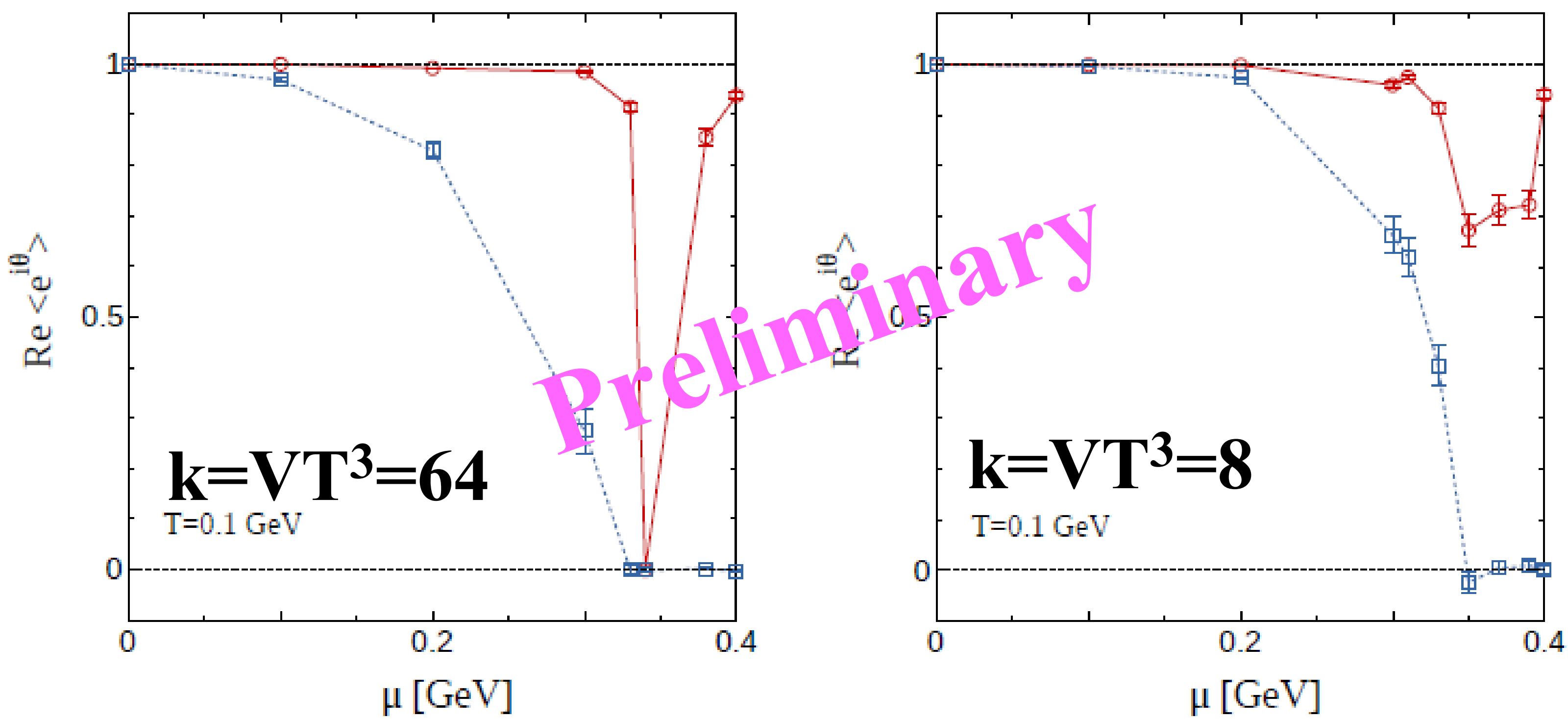
- **Action of PNJL model with vector coupling**

$$\Gamma_{\rm PNJLv} = \Gamma_{\rm PNJL} + G_v \int d^4x \left[(\bar{q}\gamma_0 q)^2 - (\bar{q}\gamma_i q)^2 \right]$$

$$\simeq -\log\det D + \int d^4x (G(\sigma^2 + \vec{\pi}^2) + G_v \omega_\mu^2) + \frac{V}{T}\mathcal{V}_\Phi(\Phi, \bar{\Phi})$$

$$D = -i\,\not{D} + m_0 + 2G\sigma - \gamma_0(\mu \underline{- 2iG_v\omega_4}) - 2iG\gamma_5\vec{\pi}\cdot\vec{\tau} + 2G_v\gamma_i\omega_i$$

Wick rotated vector field → Complex Action



K. Kashiwa, Y. Mori, AO, in prep.

Discussions

Frequently Asked Questions

- **How many parameters do you have ?**
  → Many ;) For generic trial funciton (V= # of variables)

$$y_i = y_i(x_1, x_2, \dots x_V)$$

$$N_{\rm par} = (N_{\rm layer} + 1) \times V \times (N_{\rm unit} + 1) + 2V$$

- **How about the numerical cost ?**
  → A lot ;) Derivative of J with respect to parameters cost most.

$$\frac{\partial J}{\partial c_i} = J \frac{\partial J^{-1}_{jk}}{\partial z_l} \frac{\partial z_l}{\partial c_i} \to \mathcal{O}(V^3)$$

- **It is still polynomial.**
  Does the sign problem becomes "P" problem?
  → No. The average phase factor is still exp(-# V).
  If extrapolation is possible from finite V, we have a hope.

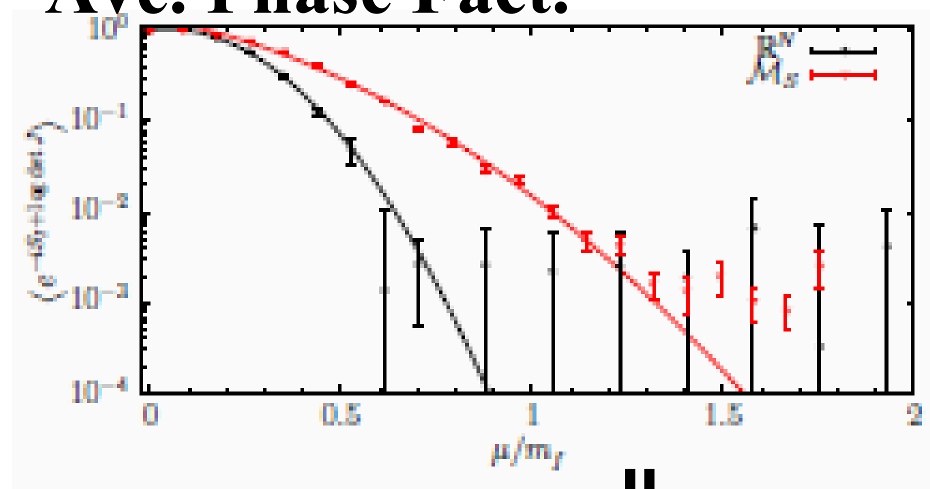
- **How can we reduce the cost ? → Next page**

How can we reduce the numerical cost ?

- **Restrict the function form of y(x).**
  - **Imaginary part is a function of its real part.**
    E.g. Alexandru, Bedaque, Lamm, Lawrence, PRD97('18)094510
    Thirring model, 1+1D QED

$$y_i = f(x_i), f(x) = \lambda_0 + \lambda_1 \cos x$$

Ave. Phase Fact.

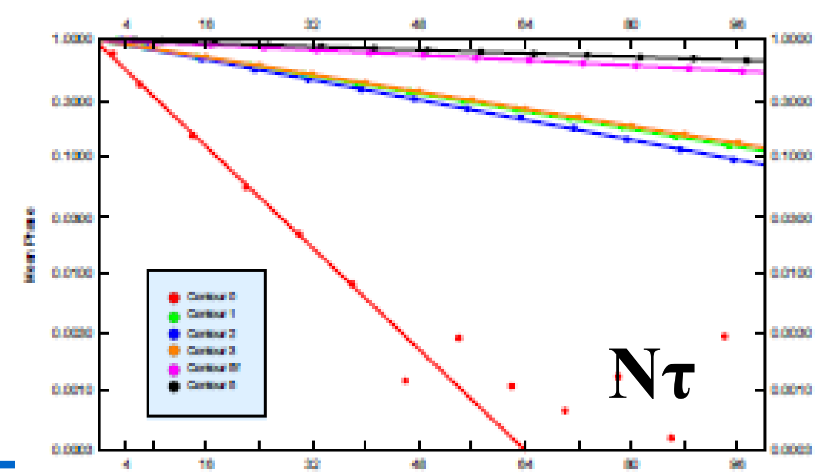


μ

  - **Nearest neighbor site**
    F. Bursa, M. Kroyter, arXiv:1805.04941
    0+1 D φ^4 theory
    Translational inv. + U(1) sym.

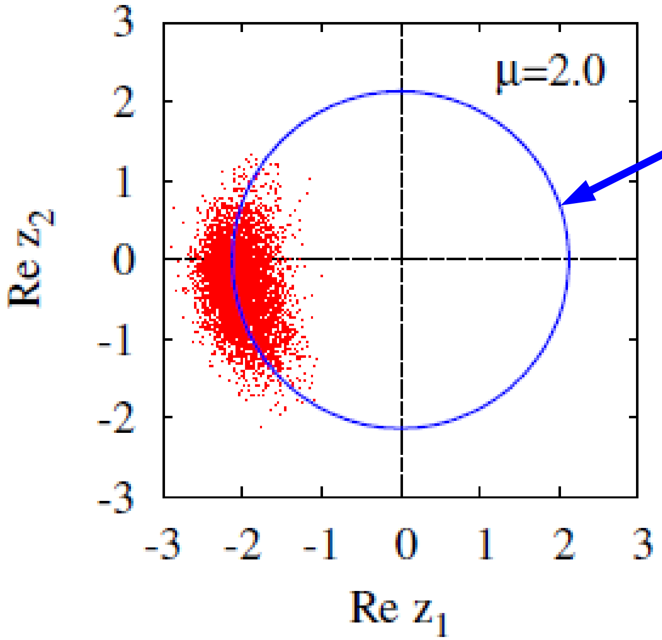
$$y_{a,i} = \frac{\varepsilon_{ab} x_{a,i+1}}{1 + x_{1,i}^2 + x_{2,i}^2}$$

Ave. Phase Fact.



Frequently Asked Questions (cont.)

- **What happens when we have 10^{10} fixed points ?**
  → In that case we should give up. (My answer @ Lattice 2017)
  → If those fixed points are connected by the symmetry, we may be able to perform path optimization.



Mean field results
= Degenerate fixed points
(All have the same θ.)

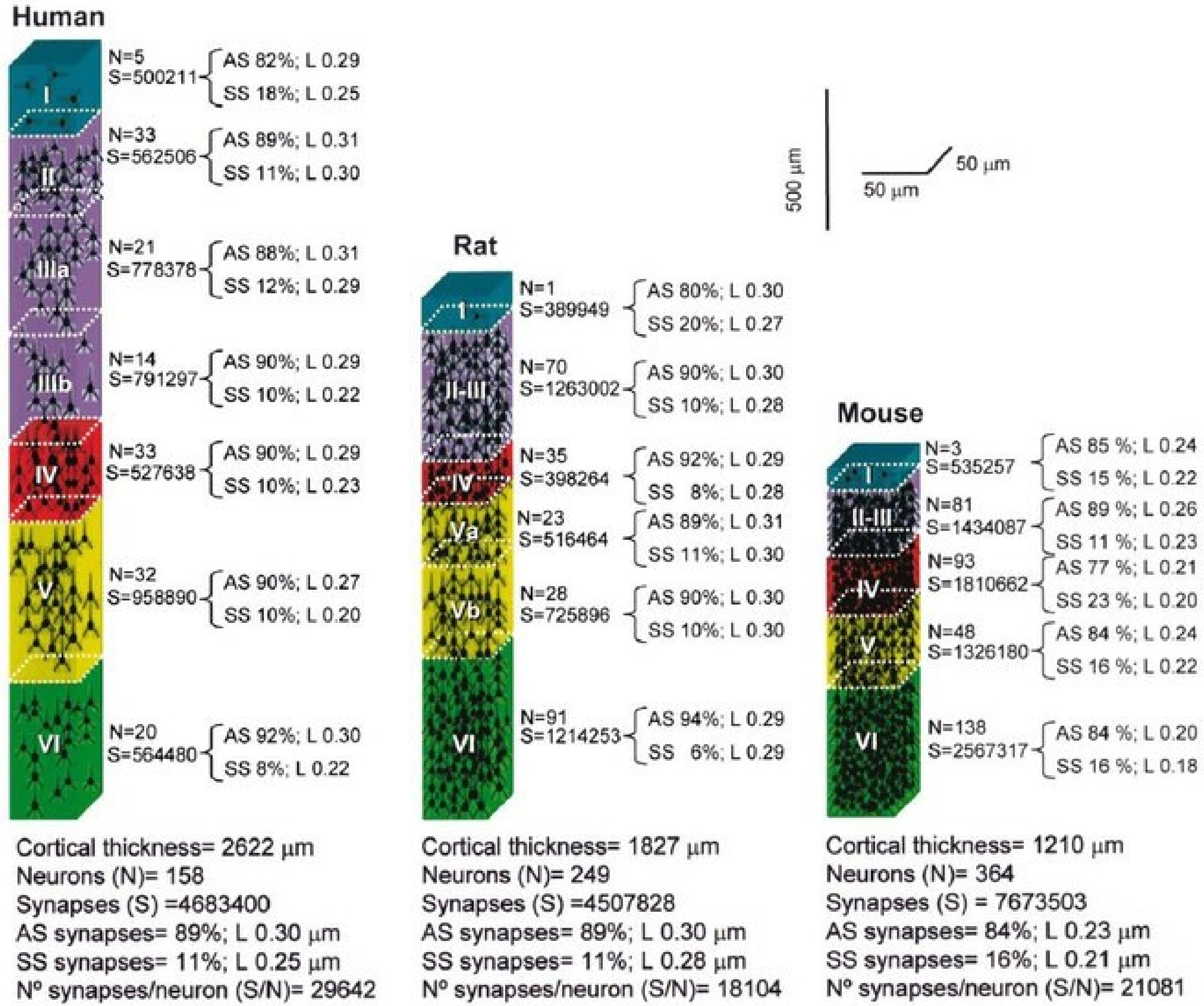
If they have different complex phases, the global sign problem emerges and the partition function would be almost zero.
E.g. H. Fujii, S. Kamata, Y. Kikukawa, arXiv:1710.08524

Summary

- The sign problem is a grand challenge in theoretical physics, and appears in many fields of physics.
  Complexified variable methods (CLM, LTM, GTM, POM) would be promising to evade the sign problem.
- Path optimization with the use of the neural network is demonstrated to work in field theories having many variables.
  - 1+1D φ^4 theory at finite μ (neural network)
  - 0+1D QCD w/ fermions (2D mesh, neural network)
  - 3+1D homogeneous PNJL (neural network)
- Neural network (single hidden layer) is the simplest device of machine learning, and it helps us to generate and optimize generic multi-variable functions, $y_i = y_i(\{x\})$.
- Gauge fields (link variables or Polyakov loop) and Repulsive interaction makes the sign problem more severe.

Layers in Human Brain

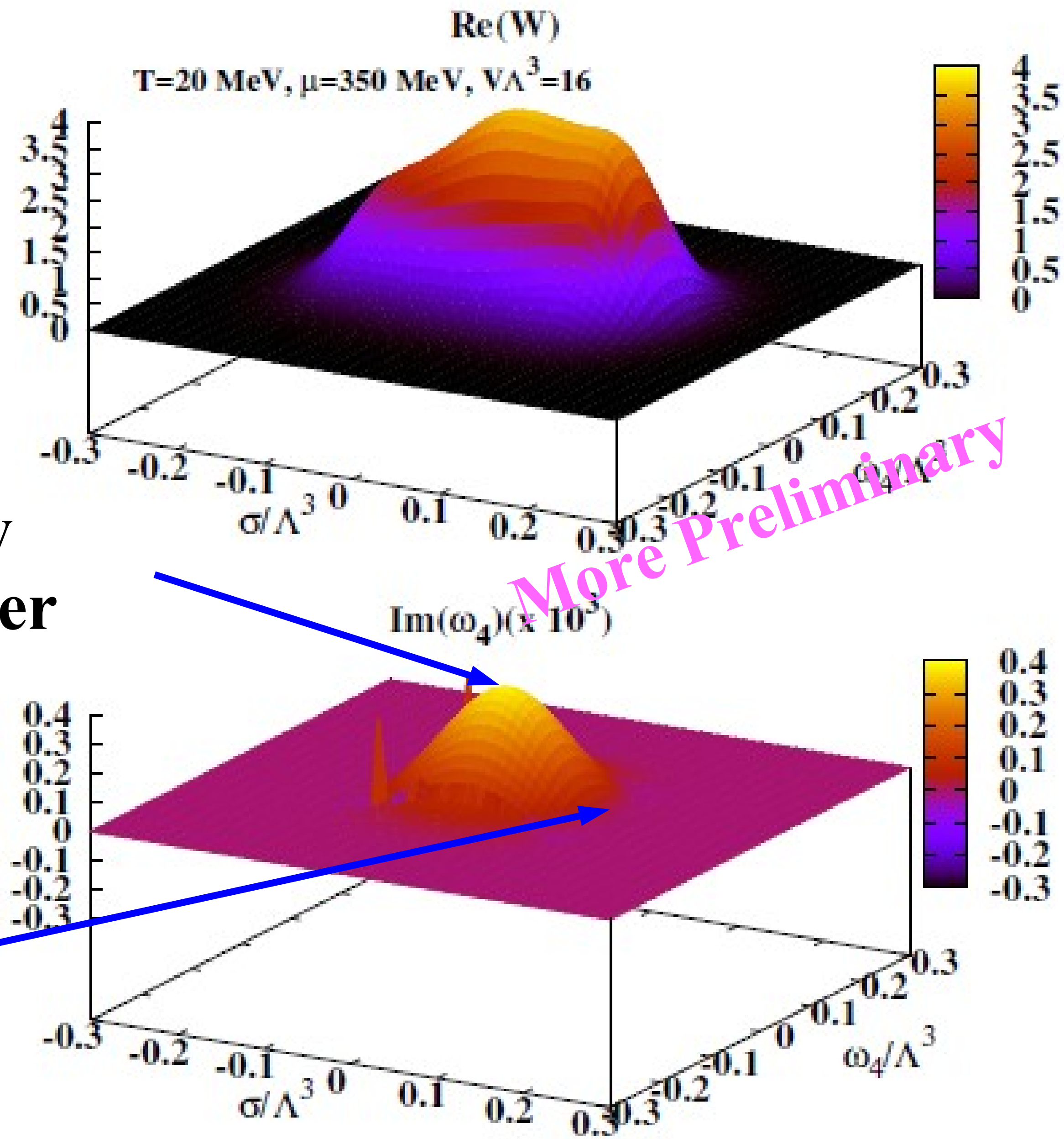
- **Defelipe 2011a (Review). The evolution of the brain, the human nature of cortical circuits, and intellectual creativity. Front Neuroanat 5, 29.**



Config. dep. vector field shift ?

High density
Quark Matter

Low density
Nuclear Matter



Application to Gauge Theory: 1 dimensional QCD

Y. Mori, K Kashiwa, AO, in prep.

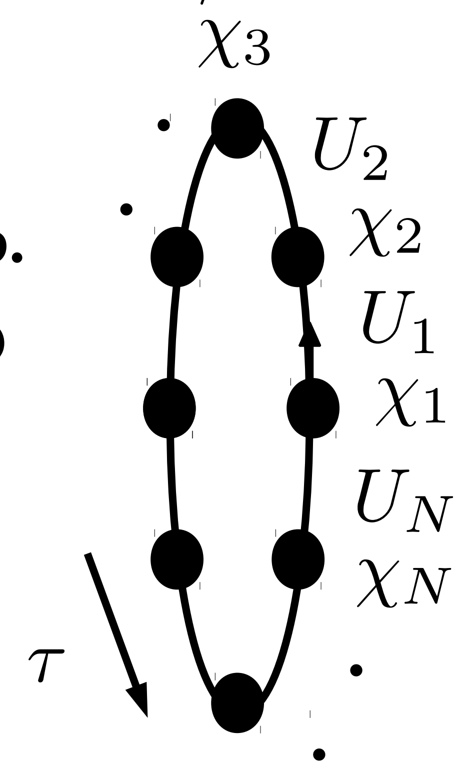
- **0+1 dimensional QCD (1 dim. QCD) with one species of staggered fermion on a 1xN lattice**

$$S = \frac{1}{2}\sum_\tau \left(\bar{\chi}_\tau e^{\mu} U_\tau \chi_{\tau+\hat{0}} - \bar{\chi}_{\tau+\hat{0}} e^{-\mu} U_\tau^{-1} \chi_\tau\right) + m \sum_\tau \bar{\chi}_\tau \chi_\tau = \frac{1}{2}\bar{\chi} D \chi$$

$$\mathcal{Z} = \int \mathcal{D}U \det D[U] = \int dU \det\left[X_N + (-1)^N e^{\mu/T} U + e^{-\mu/T} U^{-1}\right]$$

$$X_N = 2\cosh(E/T)\ ,\ E = \mathrm{arcsinh}\, m\ ,\ U = U_1 U_2 \cdots U_N\ ,\ T = 1/N$$

Bilic+('88), Ravagli+('07), Aarts+('10, CLM), Bloch+('13, subset), Schmidt+('16, LTM), Di Renzo+('17, LTM)



  - **A toy model, but the actual source of QCD sign prob.**
  - **Studied well in the context of strong coupling LQCD**
    E.g. Miura, Nakano, AO, Kawamoto('09,'09,'17), de Forcrand, Langelage, Philipsen, Unger ('14)

1 dim. QCD in diagonal gauge

- **Diagonal gauge**

$$U = (e^{iz_1}, e^{iz_2}, e^{iz_3}) \quad (z_1 + z_2 + z_3 = 0)$$

$$\mathcal{Z} = \int dU e^{-S(U)} = \int_{\mathbb{R}} dx_1 dx_2 H(x) e^{-S(x)} = \int_{\mathbb{C}} dz_1 dz_2 H(z) e^{-S(z)}$$

$$= \int dx_1 dx_2 \det\left(\frac{\partial z_a}{\partial x_b}\right) \left[\frac{8}{3\pi^2} \prod_{a<b} \sin^2\left(\frac{z_a - z_b}{2}\right)\right] \left[\prod_a (X_N + 2\cos(z_a - i\mu))\right]$$

Jacobian **Haar measure** **exp(-S)**

- **Path optimization (t: ficticious time)**
  → $y(x_1,x_2)$ itself is the parameter on the (x_1,x_2) mesh point

$$z_i = x_i + iy_1,\ y_i = y_i(x_1, x_2)$$

$$\frac{dy_i}{dt} = -\frac{\partial \mathcal{Z}_{\mathrm{pq}}}{\partial y_i},\ \mathcal{Z}_{\mathrm{pq}} = \int dx_1 dx_2 |JH\, e^{-S}|$$

Path Opt. of 1 dim. QCD in diagonal temporal gauge

- **Path optimization**
  - **Average phase factor > 0.99 → Easily achieved**
  - **exp(-S) and Haar Mesure → "six pads"** *Schmidt+('16, LTM)*

APF

fictitious time

Mori, Kashiwa, AO, in prep.

1 dim. QCD with Hybrid MC

- **Concern…**
  - **Six pads are separated by the Haar measure barrier.**

$$\text{Symmetry}: \quad S(-z) = (S(z^*))^*, z_i \leftrightarrow z_j (i, j = 1, 2, 3)$$

Do we need exchange MC or different tempering ?
E.g. Fukuma, Matsumoto, Umeda ('17)

- **Hybrid Monte-Carlo in 1 dim. QCD**

$$U \to \mathcal{U}(U) = U \prod_{a=1}^{N_c^2-1} e^{-y_i \lambda_i / 2}, \quad H = \frac{P^2}{2} + \mathrm{Re}(S(\mathcal{U}(U))$$

SL(3)

  - **8 variables → path optimization using Neural Network**

1 dim. QCD with Hybrid MC

- **HMC + diagonalization of the link**
  → All six pads are visited, and no Ex. MC needed.

Mesh point + Grad. Desc.

HMC + NN

Mori, Kashiwa, AO, in prep.