Evading the model sign problem in the PNJL model with repulsive vector-type interaction via path optimization

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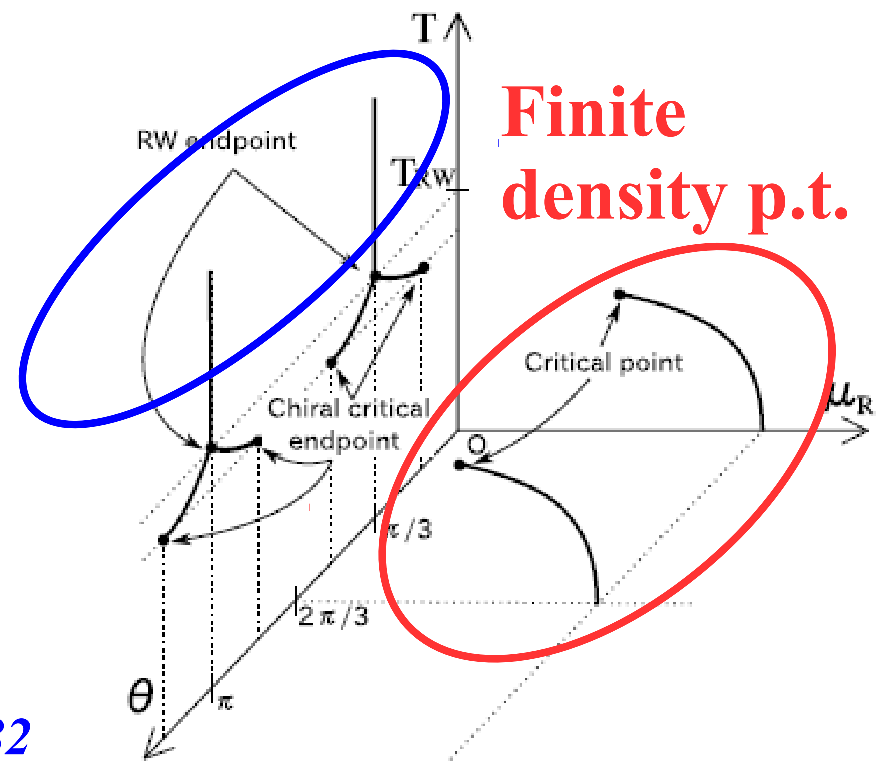
What is the nature of finite density QCD phase transition ?

- **First order phase transition boundary may exist at finite Re μ_B**
- **First order p.t. boundaries EXIST at θ=Im $\mu_q/T=\pi/3, \pi, 5\pi/3, ...$**
  → Roberge-Weiss (RW) phase transition
  [c.f. Philipsen (Tue, plenary)]

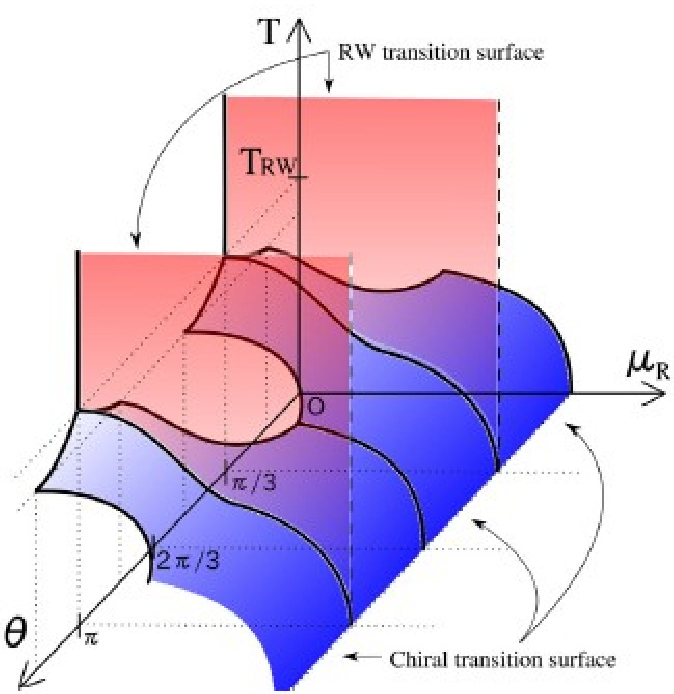
Z_3 origin
→ Deconfinement



Kashiwa, AO, PLB750 ('15) 282

Conjectured 3D phase diagram in (T, Re μ_B, θ) space

- **RW & finite density transition are CONNECTED**
  → Deconfinement assisted chiral phase transition
- **or These two are DISCONNECTED**
  → Independent of RW (deconf.) transition



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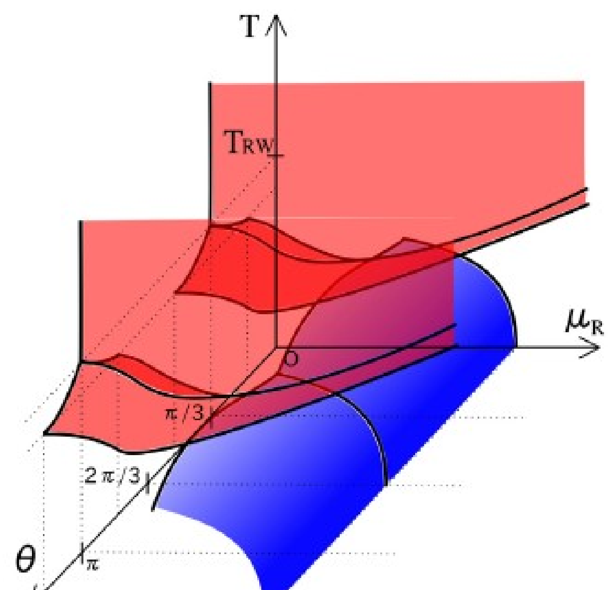


Which is true ?
PNJL (Polyakov loop extended NJL) model should give answer,
but has the sign problem at complex μ_B !

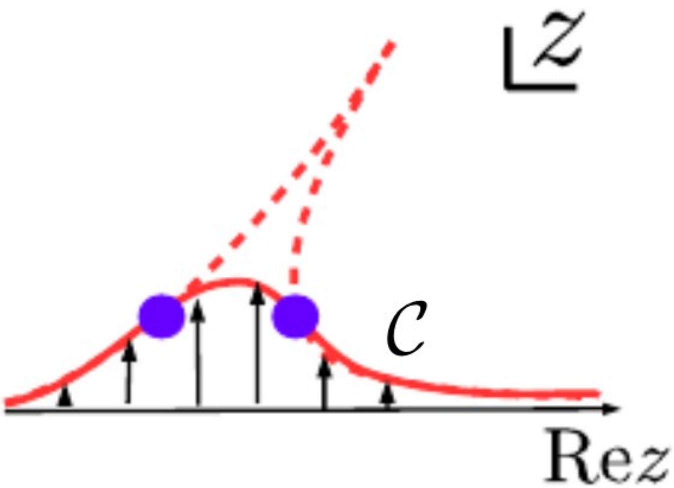
Outline

- **Introduction**
  Nature of finite density phase transition
  and the phase diagram in (T, Re μ_B, θ) space
- **Path Optimization Method**
- **Variational method & Euler-Lagrange equation for the path**
- **Example of repulsive vector-type interaction: One-site Hubbard model**
- **Application to Polyakov loop extended NJL (PNJL) model with repulsive vector-type interaction at real μ**
- **Average phase factor and Observables**
- **Configurations on Optimized Path**
- **Summary and Outlook**

Path Optimization Method

Complexified variable methods for the sign problem

- **Lefchetz thimble method**
  Witten ('10), Cristoforetti et al. (Aurora)('12), Fujii et al. ('13), Alexandru et al. ('16)
- **Complex Langevin method**
  Parisi ('83), Klauder ('83), Aarts et al. ('11), Nagata et al. ('16).
- **Path Optimization method**
  Mori+('17,'18,'19), Kashiwa+('19,'19), AO+('17,'18),
  Alexandru+('17, '18, '18), Bursa, Kroyter ('18)
  - **Integration path is variationally optimized to enhance the average phase factor.**



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

Jacobian $\det(\partial z_i/\partial x_j)$ — Complex Action — path $z = x + iy(x)$

Euler-Lagrange equation for the integral path

- **Maximizing APF = Minimizing phase quenched partition fn.**

$$\mathcal{Z}_{\rm pq} = \int d^N\varphi_R \left|\det\left(\delta_{ij} + i\frac{\partial\varphi_{j,I}}{\partial\varphi_{i,R}}\right)\exp[-S(\varphi_R + i\varphi_I)]\right|$$

$$= \int d^N x\,|W(x_i + iy_i, \partial_i y_j)| \quad (\varphi = x + iy(x))$$

- **Stationary condition of Z_{pq} w.r.t. y(x) → Euler-Lagrange eq.**

$$\frac{\delta}{\delta y_j}\mathcal{Z}_{\rm pq} = 0 \to \left[\frac{\partial}{\partial x_i}\frac{\partial}{\partial(\partial_i y_j)} - \frac{\partial}{\partial y_j}\right]|W(x+iy,\partial y)| = 0$$

- **One variable Euler-Lagrange equation**

$$\ddot{y} = (1+\dot{y}^2)^2\left[\frac{\partial({\rm Im}S)}{\partial x} + \frac{\dot{y}}{1+\dot{y}^2}\frac{\partial({\rm Re}S)}{\partial x}\right] \quad (\dot{y} = dy/dx, \ddot{y} = d^2y/dx^2)$$

Example of repulsive vector-type interaction

- **One-Site Hubbard model (strong coupling limit → Hopping term=0)**

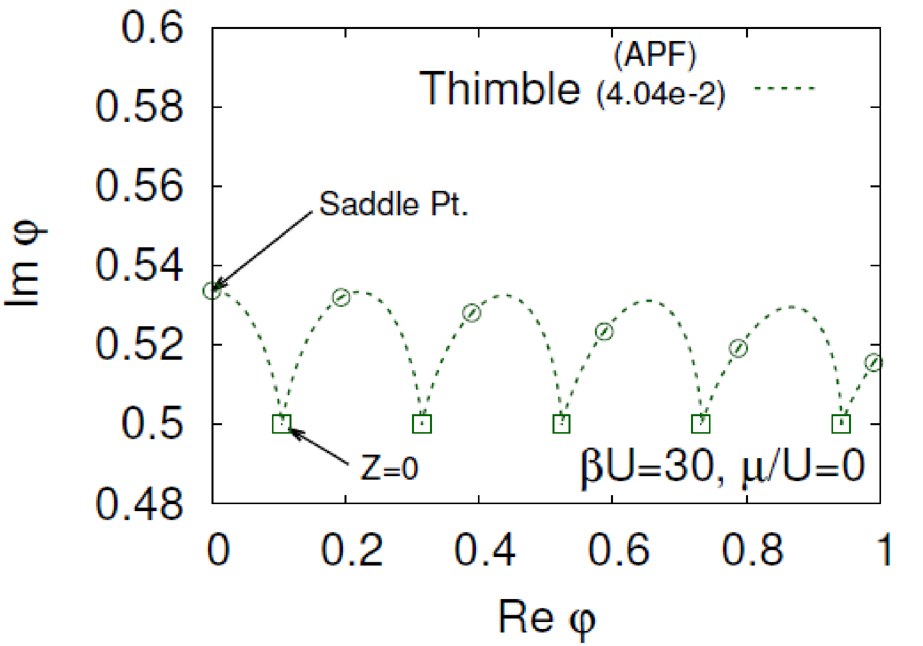
$$S = U n_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow) \quad (n_i = \psi_i^\dagger \psi_i)$$

- **Path integral representation** *Tanizaki, Hidaka, Hayata ('16)*

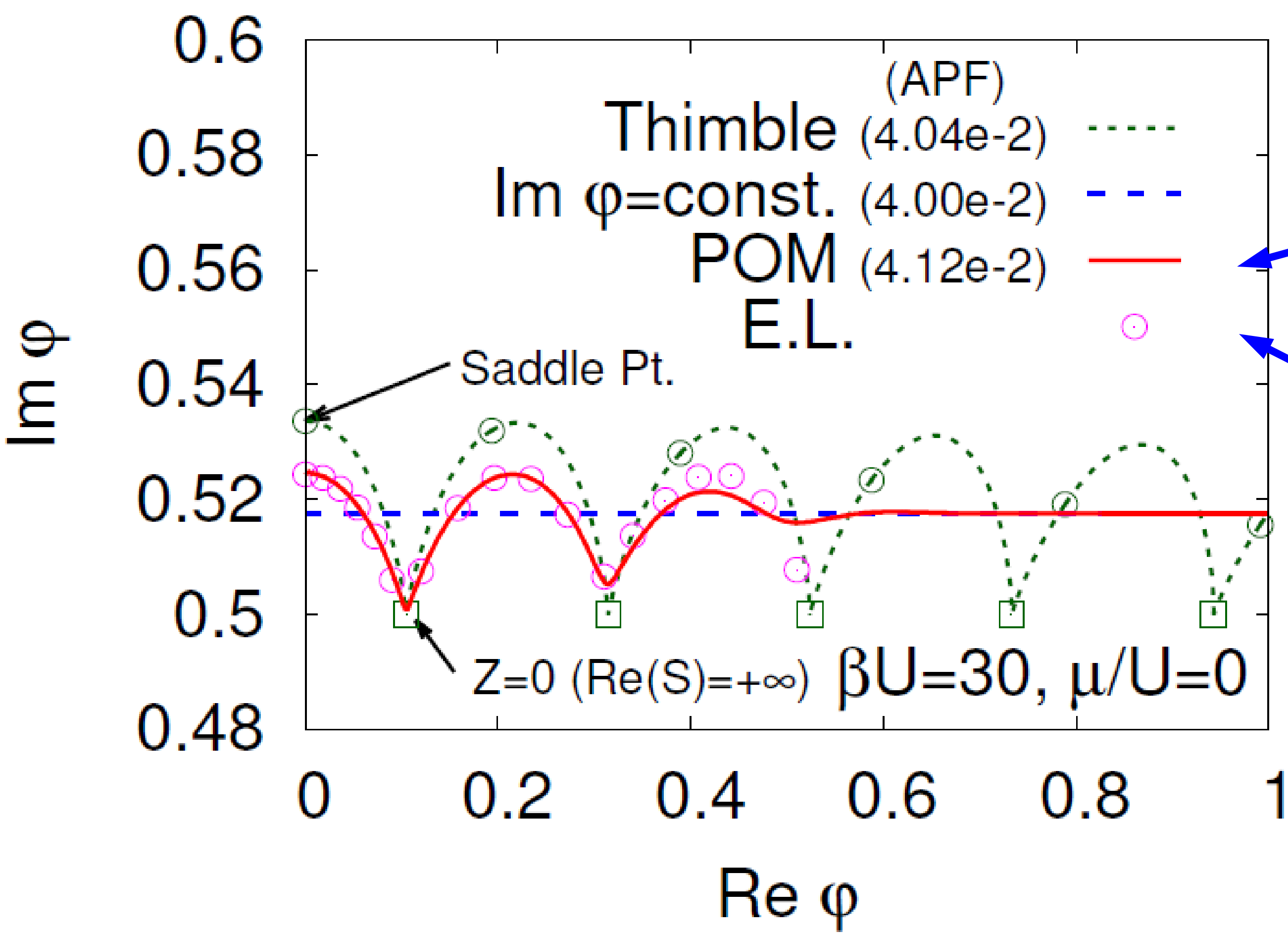
$$\mathcal{Z} = \sqrt{\frac{\beta U}{2\pi}} \int d\varphi \, [1 + \exp(\beta U(i\varphi + \mu/U + 1/2))]^2 \exp[-\beta U \varphi^2/2]$$

Complex !

- **Cancellation among multi-thimbles, and # of thimbles increases with β = 1/T**



Example of repulsive vector-type interaction



Variational POM

Solution of EL eq.

POM works also in multi-thimble prb.

AO, Mori, Kashiwa, in prep.

Application to PNJL

PNJL model

- **Polyakov-loop extended Nambu–Jona-Lasinio model**

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

- **Hubbard-Stratonovich transformation**

$$\mathcal{L}_{\text{eff}} = \bar{q}(\not{D} + m_0)q - 2G\left[\bar{q}\sigma q + \bar{q}i\gamma_5\boldsymbol{\pi}\cdot\boldsymbol{\tau}q)\right] + \mathcal{V}_g(\Phi, \bar{\Phi}) + G(\sigma^2 + \boldsymbol{\pi}^2) + 2iG_v\omega_4\bar{q}\gamma_4 q + G_v\omega_4^2$$

- **Model sign problem arises from Polyakov loop & Vector field → Ansatz !**
- **CK symmetry ansatz** *Nishimura,Ogilvie,Pangeni('14,'15)* $\mathrm{Im}A_4^3 = 0, \mathrm{Re}A_4^8 = 0$
- **Vector field (MF)** $\omega_4 = -i\rho_q$

Are these ansatz justified ?

Path Optimization in PNJL

- **Truncation of aux. field only with k=0 (Homogeneous field ansatz)**

$$\mathcal{Z} = \int \prod_{\boldsymbol{k}} dz_{\boldsymbol{k}} e^{-\Gamma(z)} \simeq \int dz_{\boldsymbol{0}} e^{-\Gamma(z_{\boldsymbol{0}})}, \quad \Gamma = \beta V \mathcal{V}_{\mathrm{eff}} = \frac{k}{T^4} \mathcal{V}_{\mathrm{eff}}$$

z=auxiliary fields & gauge field

Cristoforetti, Hell, Klein, Weise ('10)

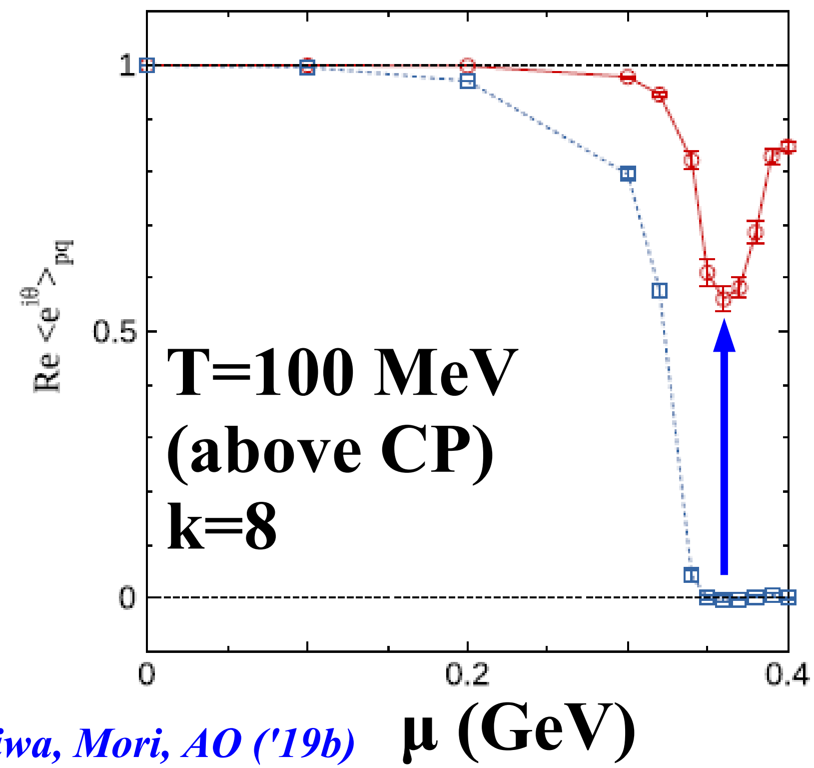
- **Variables (7 dyn. + 3 dep.)**

$$x = (\sigma, \pi^{0,+,-}, \mathrm{Re}A_3, \mathrm{Re}A_8, \mathrm{Re}\omega_4)$$

$$y = (\mathrm{Im}A_3, \mathrm{Im}A_8, \mathrm{Im}\omega_4) \ \text{(Complexified)}$$

- **Path Optimization**
  - **HMC for x (H=Re S) → 80k configs.**
  - **Mono hidden layer neural network**

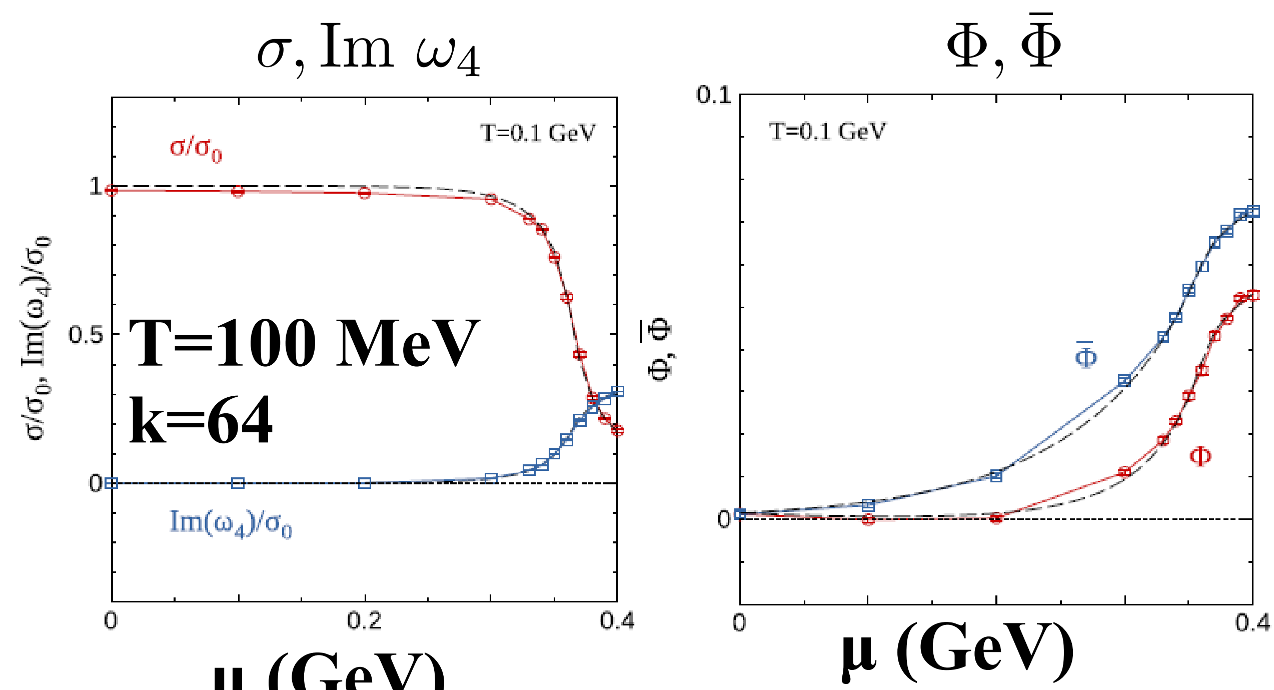
APF



Kashiwa, Mori, AO ('19b)

Observables

- μ dependence of order parameters
  - Rapid change around μ = 370 MeV (transition region)
  - Results agree with MF results under ansatz in the large space-time volume region
    → Supports these ansatz



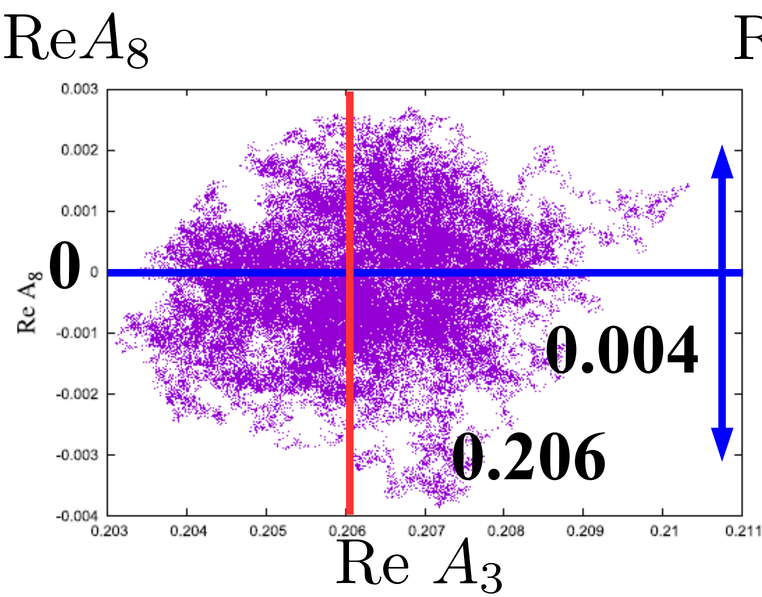
Kashiwa, Mori, AO ('19b)

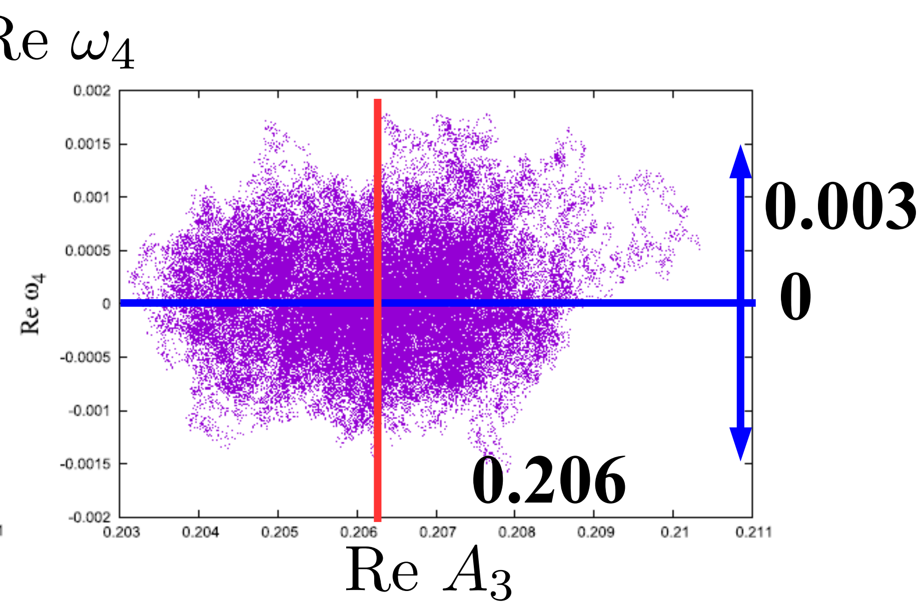
Configurations

- **Obtained configurations after training the neural network**
- **Configs. are well localized at around** $\mathrm{Re}\ A_8 = 0, \mathrm{Re}\ \omega_4 = 0, \mathrm{Re}\ A_3 \neq 0$
  $\rightarrow$ **Confirms CK symmetry and standard MF ansatz**

$$\mathcal{CK}\ \text{symmetry ansatz:} (\theta_1, \theta_2, \theta_3) = (\theta - i\psi, -\theta - i\psi, 2i\psi)$$

$$\text{MF ansatz: } \omega_4 = i\rho_q, \mathrm{Re}\ \omega_4 = 0$$





Kashiwa, Mori, AO ('19b)

Summary

- QCD phase diagram at complex μ should be useful to understand the nature of QCD phase transition. Partition fn. is an holomorphic fn. of μ with some cuts, with cuts being the 1st order p.t. boundary.
- Path optimization method is a kind of Jacobian-phase improved Lefshetz thimble method, and is flexible enough to cover the multi-thimble manifold.
- Do not care too much about # of thimbles. Care more about integrating wide enough range in the complexified field variables.
- Euler-Lagrange eq. for the path is derived, and the variational path is confirmed to agree with the solution of EL equation in the one-site Hubbard model.
- Polyakov-loop extended Nambu–Jona-Lasino model with repulsive vector-type interaction is studied in the path optimization method.
- CK sym. ansats (gluons) and mean field (vector field) ansatzs' have been confirmed in the path integral formulation. The latter is done for the first time.
- Ready to study QCD phase diagram in PNJL at complex μ.

Thank you for your attention !

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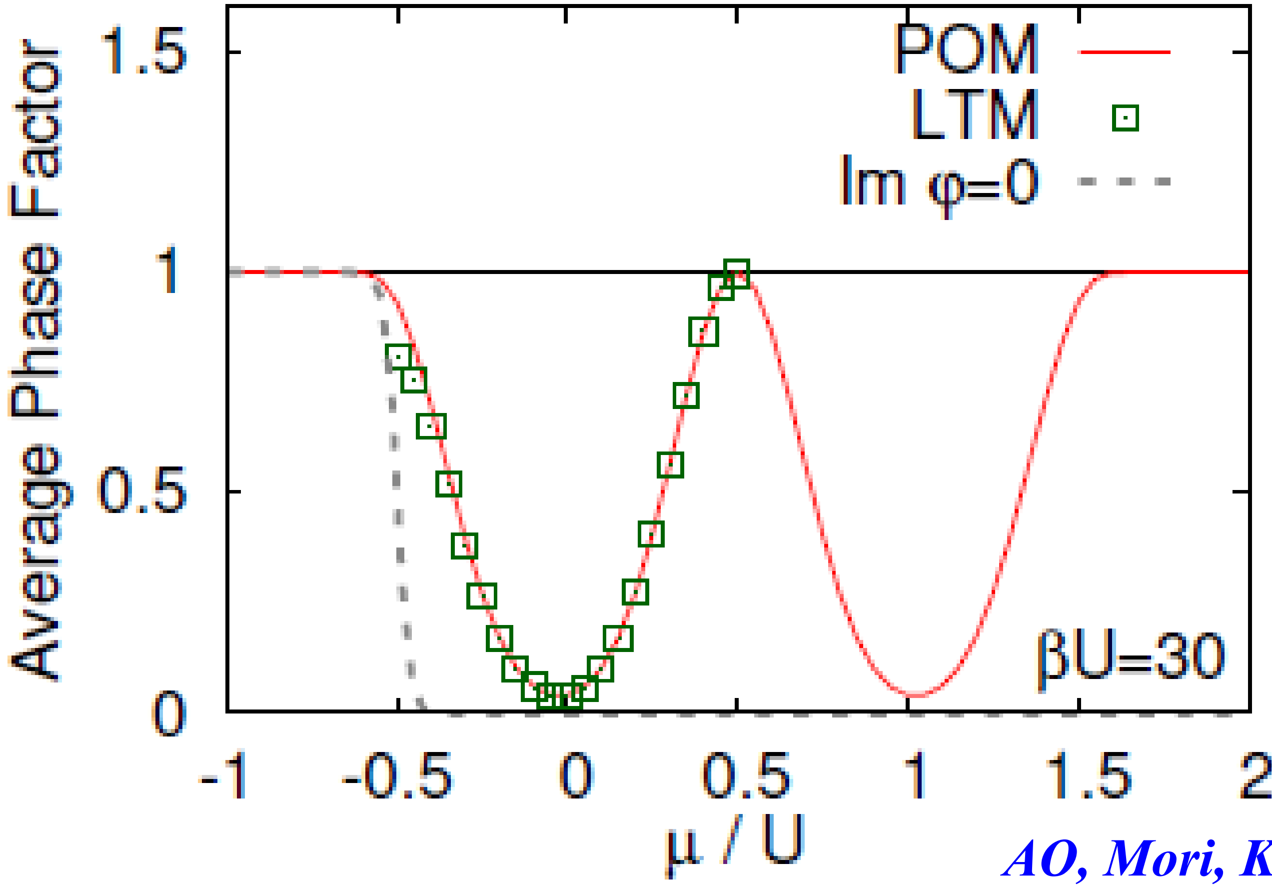
AO (11 yrs ago)

Y. Mori (grad. stu.)

K. Kashiwa (main contributor in PNJL)

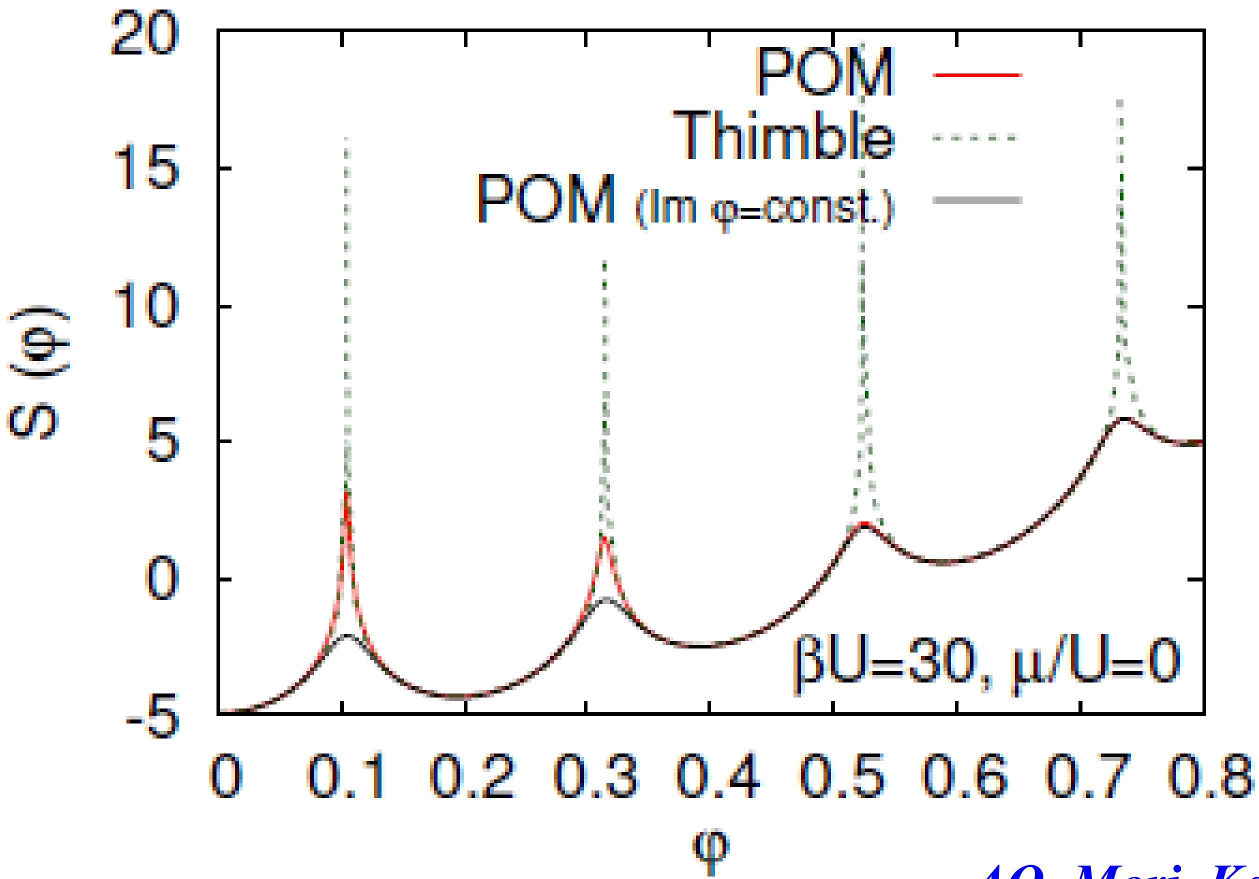
1D integral: Y. Mori, K. Kashiwa, AO, PRD 96 ('17), 111501(R) [arXiv:1705.05605]
φ4 w/ NN: Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [arXiv:1709.03208]
Lat 2017: AO, Y. Mori, K. Kashiwa, EPJ Web Conf. 175 ('18), 07043 [arXiv:1712.01088]
NJL thimble: Y. Mori, K. Kashiwa, AO, PLB 781('18),698 [arXiv:1705.03646]
PNJL w/ NN: K. Kashiwa, Y. Mori, AO, PRD 99 ('19), 014033 [arXiv:1805.08940]
PNJL w/ Vector + NN: K. Kashiwa, Y. Mori, AO, PRD 99 ('19) 114005 [arXiv:1903.03679]
0+1D QCD: Y. Mori, K. Kashiwa, AO, arXiv:1904.11140
1+1D QCD: Y. Mori, K. Kashiwa, AO, in prep., 0+1D Hubbard: AO, Mori, Kashiwa, in prep.

One-site Hubbard model



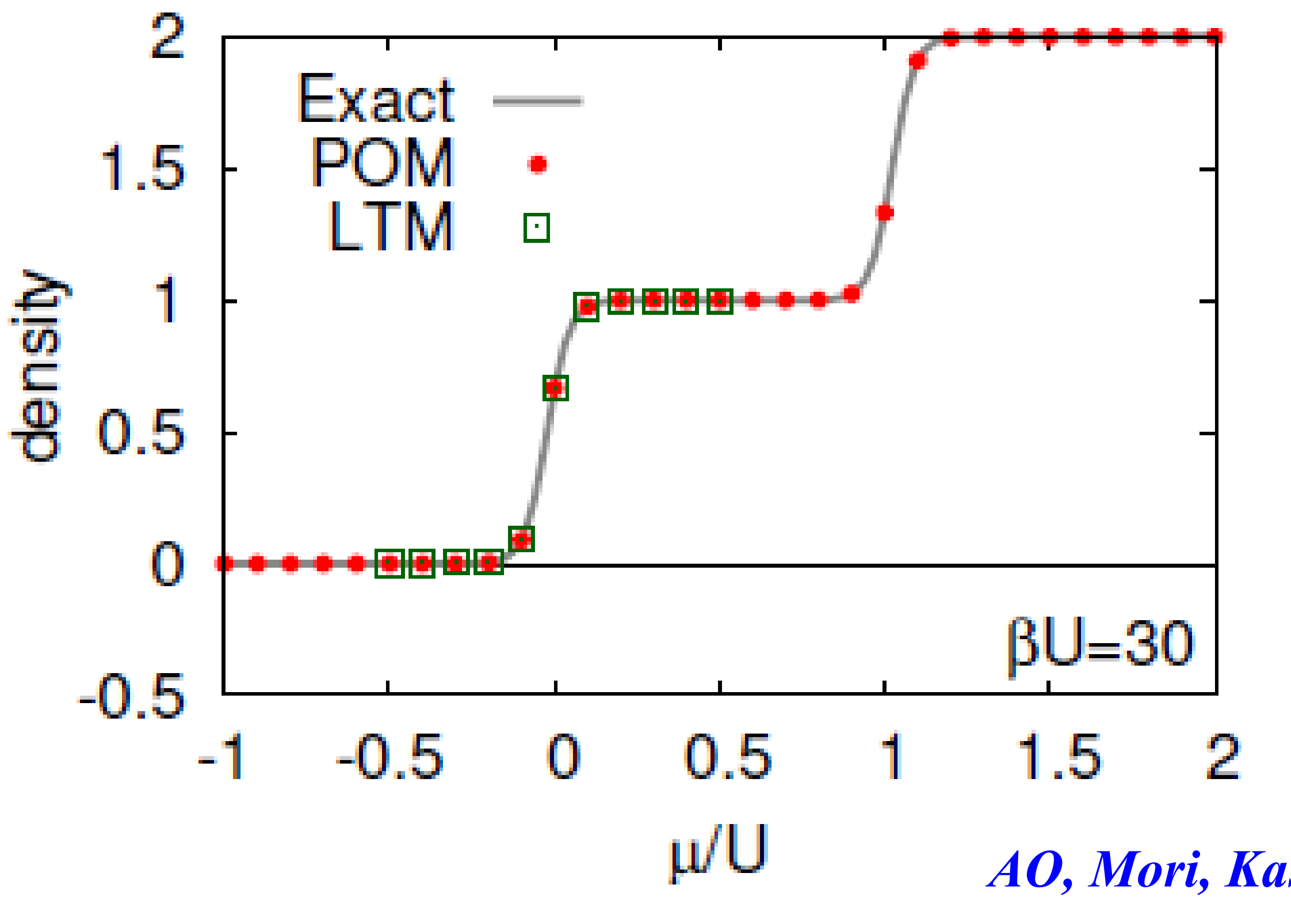
AO, Mori, Kashiwa, in prep.

One-site Hubbard model



AO, Mori, Kashiwa, in prep.

One-site Hubbard model



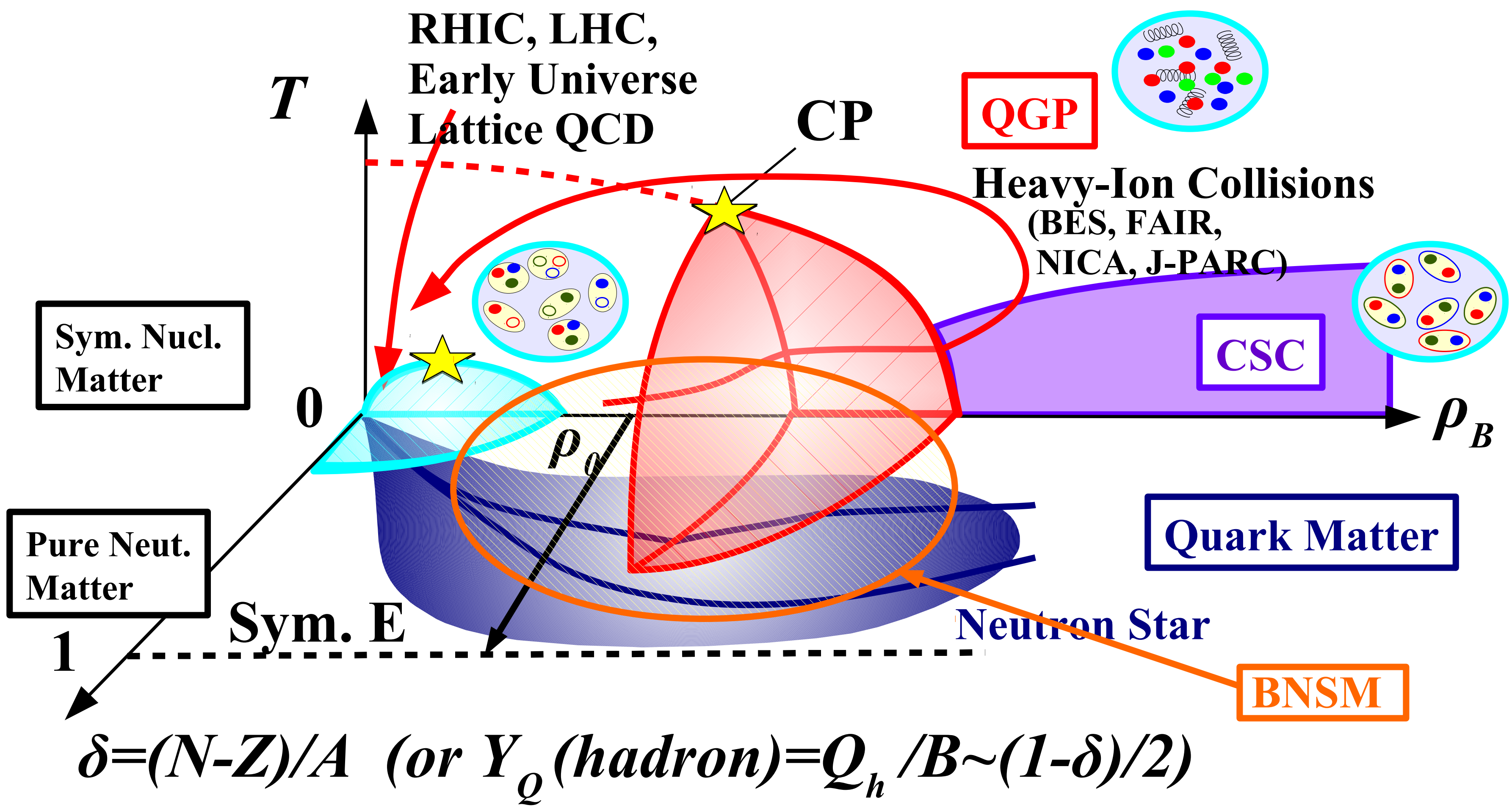
AO, Mori, Kashiwa, in prep.

Extended Hubbard-Stratonovich Transformation

$$e^{\alpha AB} = \int d\varphi\, d\phi\, e^{-\alpha\left\{(\varphi-(A+B)/2)^2+(\phi-i(A-B)/2)^2\right\}+\alpha AB}$$
$$= \int d\varphi\, d\phi\, e^{-\alpha\left\{\varphi^2-(A+B)\varphi+\phi^2-i(A-B)\phi\right\}} \,. \qquad (44)$$

Miura, Nakano, AO, Kawamoto, PRD80 (2009) 074034

QCD phase diagram



AO, JPS Conf. Proc. 20 (2018), 011035