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

Akira Ohnishi ¹, Yuto Mori ², Kouji Kashiwa ³
¹. Yukawa Inst. for Theoretical Physics, Kyoto U.,

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What is the nature of finite density QCD phase transition?

First order phase transition boundary may exist at finite $\text{Re } \mu_B$

First order p.t. boundaries EXIST at $\theta = \text{Im } \mu_q / T = \pi/3, \pi, 5\pi/3, ...$

→ Roberge-Weiss (RW) phase transition  
[c.f. Philipsen (Tue, plenary)]

$Z_3$ origin  
→ Deconfinement

Kashiwa, AO, PLB750 ('15) 282
Conjectured 3D phase diagram in \((T, \text{Re } \mu_B, \theta)\) space

- RW & finite density transition are CONNECTED
  
  -> Deconfinement assisted chiral phase transition

- or These two are DISCONNECTED
  
  -> Independent of RW (deconf.) transition

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

- Introduction
  - Nature of finite density phase transition and the phase diagram in \((T, \text{Re } \mu_B, \theta)\) 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 \(\mu\)
  - 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.

\[
\text{APF} = \langle e^{i\theta} \rangle_{pq} = \frac{\int_C dx J e^{-S}}{\int_C dx |J e^{-S}|} = \mathcal{Z} / \mathcal{Z}_{pq}
\]

- 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.

\[ Z_{pq} = \int d^N \varphi_R \det \left( \delta_{ij} + i \frac{\partial \varphi_j, I}{\partial \varphi_i, R} \right) \exp[-S(\varphi_R + i \varphi_I)] \]

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

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

\[ \frac{\delta}{\delta y_j} Z_{pq} = 0 \rightarrow \left[ \frac{\partial}{\partial x_i} \frac{\partial}{\partial (\partial_i y_j)} - \frac{\partial}{\partial y_j} \right] |W(x + iy, \partial y)| = 0 \]

- One variable Euler-Lagrange equation

\[ \ddot{y} = (1 + \dot{y}^2)^2 \left[ \frac{\partial(\text{Im}S)}{\partial x} + \frac{\dot{y}}{1 + \dot{y}^2} \frac{\partial(\text{Re}S)}{\partial x} \right] \quad (\dot{y} = dy/dx, \ddot{y} = d^2 y/dx^2) \]
Example of repulsive vector-type interaction

- One-Site Hubbard model (strong coupling limit $\rightarrow$ 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)*
  \[ Z = \sqrt{\frac{\beta U}{2\pi}} \int d\varphi \left[ 1 + \exp(\beta U(i\varphi + \mu/U + 1/2)) \right]^2 \exp[-\beta U \varphi^2 / 2] \]

  Complex!

- Cancellation among multi-thimbles, and # of thimbles increases with $\beta = 1/T$
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

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

- Hubbard-Stratonovich transformation

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

- Model sign problem arises from Polyakov loop & Vector field → Ansatz!

  - CK symmetry ansatz
    \[ \text{Im} A_4^3 = 0, \text{Re} A_4^8 = 0 \]
    \[ \text{Nishimura, Ogilvie, Pangeni} ('14, '15) \]

  - 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)

$$Z = \int \prod_k dz_k e^{-\Gamma(z)} \simeq \int dz_0 e^{-\Gamma(z_0)}, \quad \Gamma = \beta V V_{\text{eff}} = \frac{k}{T^4} V_{\text{eff}}$$

$z$=auxiliary fields & gauge field

_Cristoforetti, Hell, Klein, Weise ('10)_

- Variables (7 dyn. + 3 dep.)

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

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

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

HMC for $x$ ($H=\Re S$) $\rightarrow$ 80k configs.

Mono hidden layer neural network

$T=100$ MeV (above CP)

$k=8$

_Kashiwa, Mori, AO ('19b)_
Observables

- μ dependence of order parameters $\sigma, \text{Im} \omega_4, \Phi, \bar{\Phi}$
  - Rapid change around $\mu = 370$ MeV (transition region)
  - Results agree with MF results under ansatz in the large space-time volume region → Supports these ansatz

![Graphs showing μ dependence of order parameters](image)

Kashiwa, Mori, AO ('19b)
Obtained configurations after training the neural network

- Configs. are well localized at around \( \text{Re } A_8 = 0, \text{Re } \omega_4 = 0, \text{Re } A_3 \neq 0 \)
- Confirms CK symmetry and standard MF ansatz

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

MF ansatz: \( \omega_4 = i\rho_q, \text{Re } \omega_4 = 0 \)
Summary

- QCD phase diagram at complex $\mu$ should be useful to understand the nature of QCD phase transition. Partition fn. is an holomorphic fn. of $\mu$ 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 $\mu$. 
Thank you for your attention!

Collaborators: Akira Ohnishi\textsuperscript{1}, Yuto Mori\textsuperscript{2}, Kouji Kashiwa\textsuperscript{3}


1D integral: Y. Mori, K. Kashiwa, AO, PRD 96 ('17), 111501(R) [arXiv:1705.05605]
\(\varphi^4\) w/ NN: Y. Mori, K. Kashiwa, AO, PTEP 2018 ('18), 023B04 [arXiv:1709.03208]
NJL thimble: Y. Mori, K. Kashiwa, AO, PLB 781 ('18), 698 [arXiv:1705.03646]
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.

AO (11 yrs ago) Y. Mori (grad. stu.) K. Kashiwa (main contributor in PNJL)
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.
\[ e^{\alpha AB} = \int d\varphi \, d\phi \, e^{\alpha \left\{ (\varphi - (A+B)/2)^2 + (\phi - i(A-B)/2)^2 \right\} + \alpha AB} \]

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

Miura, Nakano, AO, Kawamoto, PRD80 (2009) 074034
QCD phase diagram

- RHIC, LHC, Early Universe
- Lattice QCD
- Heavy-Ion Collisions (BES, FAIR, NICA, J-PARC)
- QGP
- CSC
- Sym. Nucl. Matter
- Pure Neut. Matter
- Quark Matter
- Sym. E
- Neutron Star
- BNSM

\[ \delta = \frac{(N-Z)}{A} \quad \text{(or} \quad Y_Q \text{ (hadron)} = \frac{Q_h}{B} \sim (1-\delta)/2) \]

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