QCD phase diagram with both fluctuation and finite coupling effects in the strong coupling lattice QCD

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Finite density QCD and sign problem

- Finite density QCD
  - Neutron stars, Early universe, Heavy ion collisions (RHIC, LHC), ...
  - QCD phase diagram, Critical point, Inhomogeneous structure, ...

- Sign problem
  - In QCD, fermion det. becomes complex due to the chemical potential. -> breakdown of the probability interpretation
  - Approaches to finite $\mu$ region
Sign problem and representations

• The sign problem and partition function

\[ Z = \text{tr} e^{-\beta H} = \sum_n \langle n | e^{-\beta H} | n \rangle \]

• \( | n \rangle \) are eigen states of Hamiltonian: no sign problem

• \( | n \rangle \) are not eigen states of Hamiltonian: sign problem

• The sign problem depends on representation of the states.

• The representation

• How to alter representations?

• idea: converting integration procedure -> dual variables
Dual variables - 1

• Bosonic systems
  Endres, Gattringer, Schmidt, Azcoiti, …

• Fermionic systems

• Strong coupling lattice QCD (SC-LQCD)
  • Strong coupling expansion (1/g^2 expansion)
    • Expansion in plaquette terms
  • Integration procedure (different from standard Lattice QCD)
    1. link variables
    2. Grassmann variables

• Weaker sign problem in SC-LQCD compared with standard Lattice QCD
  • Effective action in terms of hadronic d.o.f.
    → We expect weaker sign problem in SC-LQCD.
  • No sign problem in the mean field (MF) approximation
  • Sign problem with fluctuation effects
• Bosonic systems
  Endres, Gattringer, Schmidt, Azcoiti, …

• Fermionic systems

**Strong coupling lattice QCD (SC-LQCD)**
**Momenr-Dimer-Polymer (MDP) simulation**

• **Integration procedure**
  1. Link variables
  2. Grassmann variables
  3. Monomer-Dimer-Polymer configurations

• **Representation**
  hadronic d.o.f.

• **Characteristics**
  1. Exact transformation from lattice QCD action in the strong coupling limit
  2. Mechanism for weakening the sign problem
     - Resummention technique
  3. Auto correlation time

• **Worm algorithm**
  
  • Strong coupling limit, Next-to-leading order by reweighing

Auxiliary field Monte-Carlo (AFMC) method

- Auxiliary field Method on QCD phase diagram in SC-LQCD

- Another way to convert representations in SC-LQCD

- Integration procedure
  1. Link variables
  2. Bosonization
  3. Grassmann variables
  (4. Auxiliary field configurations in AFMC)

- Representation
  hadronic d.o.f.

- Characteristics
  1. Manifest physical mode
  2. Manifest chiral symmetry
  3. Straightforward to include finite coupling effect

- Mean field analysis

  - Strong coupling limit, next-to-leading order, and next-to-next-to-leading order effects

  - AFMC

  - Strong coupling limit


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Finite coupling effects on QCD phase diagram in MF

- Finite coupling effects
  - To obtain the insight into the continuum limit
  - QCD phase diagram evolution (1st. order phase line)
  - To evaluate the influence on Critical point
  - Density fluctuation can be included via NLO bosonization, which is important effects on QCD critical point.

MF : Miura, Nakano, Ohnishi, Kawamoto (2009)
Nakano, Miura, Ohnishi (2011)
Reweighting: de. Forcrand et. al. (2013), Unger (2014)
Strong coupling lattice QCD
with fluctuations in the strong coupling limit (SCL)

- Fluctuation effects
  - Important step to evaluate partition function exactly

- Current numerical approaches
  - Monomer-Dimer-Polymer (MDP) simulation
  - Auxiliary field Monte-Carlo (AFMC) method

- QCD phase diagram in SCL

- Origin of sign problem
  - MDP : Baryon loop configurations
  - AFMC : Bosonization procedure

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\( \Delta f \) : the difference of the free energy density between full and phase quenched simulation
Purpose

- To develop a method to include **both**
  
  1. **finite coupling**
     (Next-to-Leading order (NLO) of strong coupling expansion here)
  
  2. **fluctuation effects**

- To discuss the sign problem in AFMC

- To investigate phase diagram evolution
Lattice QCD action

• Unrooted staggered fermion, anisotropic lattice, lattice spacing $a=1$

\[ S_{LQCD} = \frac{1}{2} \sum_{x, \nu=0}^{d} \left[ \eta_{\nu,x}^+ \bar{\chi}_x U_{\nu,x} \chi_x + \hat{\nu} - \eta_{\nu,x}^- (H.C.) \right] + \frac{m_0}{\gamma} \sum_x \bar{\chi}_x \chi_x + \frac{2N_c \xi}{g_\tau^2 (g_0, \xi)} P_{\tau} + \frac{2N_c}{g_s^2 (g_0, \xi) \xi} P_s + \frac{1}{g^2} \]

• Assuming $\gamma = \xi$ and $g_\tau = g_s$, temporal lattice spacing is expressed as $a_\tau = a / \gamma^2$ due to quantum corrections, so we here define $T = \gamma^2 / N_\tau a$.

($T_c (\mu=0)$ does not depend on aniso. parameters.)

N. Bilic et. al. (1992, 1995)
Effective action in the strong coupling limit

- $1/g^2$ expansion, leading order of $1/d$ (large dimensional) expansion

- $U_j$ (spatial link) integration

$$S_{\text{eff}} = \frac{1}{2} \sum_x [V^+_x - V^-_x] + \frac{1}{4N_c \gamma} \sum_{x,j} M_x M_{x+j} + \frac{m_0}{\gamma} \sum_x M_x$$

$$\int dU U_{ab} U_{cd}^\dagger = \frac{1}{N_c} \delta_{ad} \delta_{bc}$$

$$V_x^+ = e^{\mu a_\tau} \bar{x}_0 U_{0,x} \chi_U x \chi_{x+\hat{0}}$$

$$V_x^- = e^{-\mu a_\tau} \bar{x}_{x+\hat{0}} U_{0,x}^\dagger \chi_x$$

$$M_x = \bar{x}_x \chi_x$$
Auxiliary filed Monte-Carlo (AFMC) method

- Extended HS (EHS) transformation
  - Fluctuation effects: Different value at each site
  - Necessity to introduce complex term

\[
\exp[\alpha AB] = \int \mathcal{D}[\phi, \varphi] \exp\left[-\alpha \left\{ \phi^2 + \varphi^2 + (A + B)\varphi - i(A - B)\phi \right\}\right]
\]

- Bosonization

\[
Z = \int \mathcal{D}[\sigma, \pi] e^{-S_{\text{eff}}(\sigma, \pi)}
\]

- Modified mass

\[
m_x = m_0 + \frac{1}{4N_c} \sum_j (\sigma + i\epsilon\pi)_{x \pm j}
\]

\[
\epsilon_x = (-1)^{x_0 + \cdots + x_d}
\]
Effective action and AFMC method

**Sec. 2 Formalism**

- **Effective action (after Grassmann and $U_0$ integration) in SCL**

\[
S_{\text{eff}}^{\text{AF}} = \sum_{k, \tau, f(k) > 0} \frac{L^3 f(k)}{4N_c} \left[ |\sigma_{k,\tau}|^2 + |\pi_{k,\tau}|^2 \right] \\
- \sum_x \log \left[ X_{N_\tau} (x)^3 - 2X_{N_\tau} (x) + 2 \cosh (3N_\tau \mu / \gamma^2) \right]
\]

- **Smaller phase at larger $\mu$**

- **Auxiliary filed Monte-Carlo (AFMC) method**

\[
f(k) = \sum_{j=1}^{d} \cos k_j
\]

\[
\epsilon_x = (-1)^{x_0 + \cdots + x_d}
\]

Integration over AFs by Monte-Carlo technique

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Effective action with NLO terms

- $1/g^2$ expansion, leading order of $1/d$ (large dimensional) expansion

- $U_j$ (spatial link) integration

Formalism

\[
\int dU U_{ab} U_{cd}^\dagger = \frac{1}{N_c} \delta_{ad} \delta_{bc}
\]

\[
V_x^+ = e^{\mu \alpha \tau} \bar{\chi}_{x} U_{0,x} \chi_{x+\hat{0}} ,
\]
\[
V_x^- = e^{-\mu \alpha \tau} \bar{\chi}_{x+\hat{0}} U_{0,x}^\dagger \chi_{x} ,
\]
\[
M_x = \bar{\chi} x \chi ,
\]
Effective action with NLO terms

- $1/g^2$ expansion, leading order of $1/d$ (large dimensional) expansion

- $U_j$ (spatial link) integration

- Extended Hubbard-Stratonovich (EHS) transformation
  - spatial terms; $\text{MMMM} \rightarrow \text{MM} \rightarrow M$ (sequential bosonization)
  - temporal terms; $\text{VV} \rightarrow V$

Origin of sign problem

- $\exp[\alpha AB] = \int \mathcal{D}[\phi, \varphi] \exp \left[-\alpha \left[\phi^2 + \varphi^2 + (A + B)\varphi - i(A - B)\phi\right]\right]$
Effective action with NLO terms

- Effective action after bosonization ($\Phi$ are auxiliary fields (AFs), SCL=strong coupling limit, sp.=spatial, t.=temporal, NLO=next leading order)

$$S_{\text{eff}}^{\text{EHS}} = \frac{1}{2} \sum_x \Phi_x^2 + \sum_x m_x(\Phi) M_x$$

$$+ \frac{1}{2} \sum_x Z_x(\Phi) [V_x^+(\tilde{\mu}(\Phi)) - V_x^-(\tilde{\mu}(\Phi))]$$

- Modified mass

$$m_0 \rightarrow m_x(\Phi_{\text{SCL}}, \Phi_{\text{sp. NLO}})$$

- Modified chemical potential

$$\mu \rightarrow \tilde{\mu}_x(\Phi_{\text{t. NLO}})$$

- Wave function renormalization

$$1 \rightarrow Z_x(\Phi_{\text{t. NLO}})$$

- Grassmann & $U_0$ (temporal link) integration

- NLO effective action in terms of hadronic d.o.f.
  → Detail expressions are given in the back-up slides

- Auxiliary field Monte-Carlo (AFMC) method
  We integrate out auxiliary fields by Monte-Carlo technique

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Results and discussion

• Reservation

  • Unrooted staggered fermion \( (n_f=4 \text{ in the continuum limit}) \)

  • Anisotropic lattice

  • chiral limit

  • all results are shown in the lattice unit

• We show results of
  SCL
  t.NLO \( (\text{SCL} + \text{temp. plaq. NLO terms}) \)
  sp.NLO \( (\text{SCL} + \text{sp. palq. NLO terms}) \)
Results - strong coupling limit (SCL)

- Low $\mu/T$
  - 2nd order or crossover (would-be second)

- High $\mu/T$
  - 1st order (would-be first)
    - hysteresis
    - dependence on initial conditions
      Wigner start ($\sigma = 0.01$) and NG start ($\sigma = 2$)

$\mu/T = 0.1$
$\mu/T = 1.8$
Results - phase diagram in SCL

• Low $\mu/T$
  • Chiral susceptibility peak
  • Reduced $T_c$
  • almost no size dependence

• High $\mu/T$
  • Comparing with effective action from different initial conditions
  • Enhanced $\mu_c$
  • small spatial size dependence
  • $N\tau$ dependence

Phase diagram is consistent with MDP
Results - average phase factor in SCL

- Average phase factor
  = Weight cancellation

\[ \langle e^{i\theta} \rangle = \frac{Z_{\text{full}}}{Z_{\text{phase quenched}}} \]

- $4^4$ lattice \( \langle e^{i\theta} \rangle \geq 0.85 \)
- $8^4$ lattice \( \langle e^{i\theta} \rangle \geq 0.1 \)

\[ \mu/T=0.1 \quad \mu/T=1.8 \]
Discussion - the sign problem in SCL

• The severity of the sign problem

  • \( \Delta f = f^{\text{full}} - f^{\text{p.q.}} \), the difference of the free energy density in full and phase quenched MC simulations

  \[ e^{-L^3N_{\tau}} \Delta f = \frac{Z_{\text{full}}}{Z_{\text{p.q.}}} = \langle e^{i\theta} \rangle_{\text{p.q.}} \]

  • \( \Delta f (\text{AFMC}) \approx 1.0 \times 10^{-3} \)

  • \( \Delta f (\text{MDP}) \approx 0.5 \times 10^{-3} \)

  • AFMC has more severe weight cancellation

  • \( \Delta f (\text{AFMC}) \approx 2 \times \Delta f (\text{MDP}) \)

• Do we need to improve AFMC method for a larger lattice and finite coupling?
Discussion - source of the sign problem

- Modified mass term
  \[ m_x = m + \frac{1}{4N_c} \sum_j (\sigma + i\epsilon\pi)_{x \pm j} \]
- Momentum
  - Low momentum
    - Cancellation mechanism
  - small phase
  - High momentum
    - No cancellation mechanism

\[ \epsilon_x = (-1)^{x_0 + \cdots + x_d} \]
Discussion - auxiliary field momentum cut-off

• High momentum
  = High momentum modes of spatial kinetic momentum

• Cutting off high momentum auxiliary field components
  • Reductions of weight cancellations?

• Qualitative confirmations
  • Average phase factor goes to 1
  • Weight cancellations weaken
    e.g. $8^3 \times 8$ lattice, $\mu/T=0.6$

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Results - temporal NLO (t.NLO) effects - (1)

- Average phase factor ($\beta=0,1,3$)
  - Large enough $\langle e^{i\theta} \rangle \geq 0.9$
  - Sign problem is not serious in small lattice
- t.NLO auxiliary fields do not drastically affect average phase factor at $\mu=0$
Results - temporal NLO (t.NLO) effects - (2)

- Chiral condensate (Chiral radius) ($\beta=0,1,3$)
  - Fluctuation reduces chiral condensate compared with mean field (MF) results.
  - t.NLO auxiliary fields reduce chiral condensate compared with SCL results.
  - t.NLO AFs generate wave functional renormalization, which rescale effective mass.

Miura, Nakano, Ohnishi, Kawamoto (2009)
Nakano, Miura, Ohnishi (2011)
Results - spatial NLO (sp.NLO) effects

- Average phase factor ($\beta=0.1$)
  - Smaller than average phase factor of temporal NLO and SCL results
- Chiral condensate
  - almost the same as $\beta=0$ up to current $\beta$
  - similar to aniso. MF analysis
Summary

- We give an effective action including both finite coupling and fluctuation effects.
- In SCI, we give results of order parameters, phase diagram, and discuss the origin of the sign problem.
  - 1st order phase transition at high $\mu$, 2nd or crossover at low $\mu$
  - Sign problem comes from high momentum modes of the pion field
- We give results of NLO effects
  - From numerical results at $\mu=0$,
    - chiral condensate
      - is reduced by temporal NLO fields
      - is not altered much by spatial NLO fields
    - average phase factor
      - is large enough with temporal NLO fields
      - becomes small with spatial NLO fields
- We are developing a new way to weaken the sign problem to investigate larger $\mu$, $\beta$ and lattice in AFMC.
Results - t. NLO effects (t.NLO AFs & Z)

- AFs for t. NLO fields in MF
  - $\varphi_t : \varphi_t = -\langle V^+ - V^- \rangle / 2$
  - $\omega_t : \omega_t = -\langle V^+ + V^- \rangle / 2 = \rho_q$
    
  - Wave function renormalization $Z$
    - $Z$ at $\mu=0$ in MF
      
      
      
      $Z = (1 + \beta_t \varphi_t)$
      
      $\beta_t = d / N_c^2 g^2$
    - Rescaling modified mass
      
      $S_{\text{eff}}^{EHS} = \frac{1}{2} \sum_x \Phi_x^2 + \sum_x m_x(\Phi) M_x$
      
      $+ \frac{1}{2} \sum_x Z_x(\Phi) \left[ V_x^+(\tilde{\mu}(\Phi)) - V_x^-(\tilde{\mu}(\Phi)) \right]$

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Results - t. NLO effects (chiral condensate)

- Compared with MF results, chiral condensate is reduced by approximately 7% in SCL.

- is also reduced by approximately 7% in t.NLO.

- Surprisingly, chiral condensate is altered cumulatively by finite coupling and fluctuation effects.
NLO effective action (1)

- Auxiliary Fields (AFs)
  - SCL: $\sigma$ and $\pi$ are AFs for $M$ terms
  - spatial NLO: $\Sigma$ and $\Pi$ are AFs for $MM$ terms
  - temporal NLO: $\omega$ and $\Omega$ are AFs for $V$ terms

---

SCL

NLO

$\sigma, \pi$  $\omega, \Omega$  $\Sigma, \Pi$

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**NLO effective action (2)**

Correction to mass, $\mu$, wave function

\[
m_x = m_0 + \frac{1}{4N_c} \sum_j \left[ (\sigma + i\epsilon\pi)_{x-j} + (\sigma + i\epsilon\pi)_{x+j} \right] + C_s i \left[ (\varphi_x - i\phi_x) + \sum_j \left( C^{s}_{j,x-j}\varphi_{x-j} + iC^{s}_{j,x-j}\phi_{x-j} \right) \right]
\]

\[
e^{\mu_x} = e^\mu e^{-\delta\mu_x} = e^\mu \sqrt{\alpha^-_x / \alpha^+_x}
\]

\[
Z_x = \sqrt{\alpha^+_x \alpha^-_x}
\]

\[
C_\tau = 1/(2N_c^2 g^2 \gamma)
\]

\[
C_s = 1/(2N_c^3 g^2 \gamma)
\]

\[
C^{s}_{j,x} = C^{s}_{j,x} (\Sigma, \Pi)
\]

\[
\alpha^-_x = 1 + C_\tau \sum_j \left[ i\omega_{x\pm j} + (\epsilon\Omega)_{x\pm j} \right]
\]

\[
\alpha^+_x = 1 - C_\tau \sum_j \left[ i\omega^*_{x\pm j} + (\epsilon\Omega^*)_{x\pm j} \right]
\]
Effective action

\[ S_{\text{eff}}^{(\text{NLO})} = \frac{L^3 C_s}{8N_c} \sum_{\tau, u, \kappa_u^j > 0, j} \kappa_u^{(j)} \left[ |\Sigma_u^{(j)}|^2 + |\Pi_u^{(j)}|^2 \right] + L^3 C_T \sum_{\tau, k, f(k) > 0} f(k) \left[ |\omega_{k, \tau}|^2 + |\Omega_{k, \tau}|^2 \right] \]
\[ + \frac{L^3}{4N_c} \sum_{k, \tau, f(k) > 0} f(k) \left[ |\sigma_{k, \tau}|^2 + |\pi_{k, \tau}|^2 \right] + \frac{C_s}{4N_c} \sum_x \left[ \phi_x^2 + \varphi_x^2 \right] \]
\[ - \sum_x \log \left[ X_{N, \tau}(x)^3 - 2\hat{Z}(x)^2 X_{N, \tau} + \hat{Z}(x)^3 \cosh \left( 3\hat{\mu}(x) \right) \right]. \]

\[ C_T = 1/(2N_c^2 g^2 \gamma) \]
\[ C_s = 1/(2N_c^3 g^2 \gamma) \]
\[ C^s_{j, x} = C^s_{j, x}(\Sigma, \Pi) \]
\[ \alpha_x^- = 1 + C_T \sum_j \left[ i\omega_{x, \pm j} + (e\Omega)_x \pm j \right] \]
\[ \alpha_x^+ = 1 - C_T \sum_j \left[ i\omega_{x, \pm j}^* + (e\Omega^*)_x \pm j \right] \]
\[ f(k) = \sum_{j > 0} \cos k_j \]
\[ \kappa_u^{(j)} = \sum_{k(\neq j)} \cos u_k \]
\[ e^{\bar{\mu}_x} = e^\mu \sqrt{\alpha_x^- / \alpha_x^+} \]
\[ \hat{Z}(x) = \Pi_i Z_{x, i} \]
\[ X_N \text{ is a known function} \]
Calculation of fermion determinant

\[ \mathcal{R} = \int \mathcal{D}[\chi, \bar{\chi}, U_0] e^{-\sum_{x,y} \bar{\chi}_x G_{x,y}^{-1} \chi_y} \]

\[ = \prod_x \int \mathcal{D}U_{0,x} D\left( \begin{array}{cccc}
  I_1 \cdot 1_{N_c} & \alpha_1 \cdot 1_{N_c} & 0 & \cdots \\
  -\beta_1 \cdots 1_{N_c} & I_2 \cdot 1_{N_c} & \alpha_2 \cdot 1_{N_c} & \cdots \\
  0 & \ddots & \ddots & \ddots \\
  0 & \alpha_{N_\tau} U_{0,x} & 0 & -\beta_{N_\tau-1} \cdot 1_{N_c} \\
  \end{array} \right) D\left( \begin{array}{c}
  \beta_{N_\tau} U_0^{+} \alpha_0, x \\
  0 \\
  \alpha_{N_\tau-1} \cdot 1_{N_c} \\
  I_{N_\tau} \cdot 1_{N_c} \\
  \end{array} \right) \]
NLO effective action (5)

- Calculation of fermion determinant

\[
\mathcal{R} = \prod_x \left[ X_{N_\tau}(x)^3 - 2 \hat{Z}(x)^2 X_{N_\tau} + \hat{Z}(x)^3 2 \cosh \left( 3 \hat{\mu}(x) \right) \right]
\]

- \( X_N : X_{N_\tau}(I_1, \cdots, I_{N_\tau}; \gamma_1, \cdots, \gamma_{N_\tau}) = B_{N_\tau}(I_1, \cdots, I_{N_\tau}; \gamma_1, \cdots, \gamma_{N_\tau-1}) + \gamma_{N_\tau} B_{N_\tau-2}(I_2, \cdots, I_{N_\tau-1}; \gamma_2, \cdots, \gamma_{N_\tau-2}) \),

\[
B_{N_\tau}(I_1, \cdots, I_{N_\tau}; \gamma_1, \cdots, \gamma_{N_\tau-1}) = I_{N_\tau} B_{N_\tau-1}(I_1, \cdots, I_{N_\tau-1}; \gamma_1, \cdots, \gamma_{N_\tau-2}) + \gamma_{N_\tau-1} B_{N_\tau-2}(I_1, \cdots, I_{N_\tau-2}; \gamma_1, \cdots, \gamma_{N_\tau-3})
\]

\[
B_N(I_1, \cdots, I_N; \gamma_1, \cdots, \gamma_{N-1}) = \begin{vmatrix}
I_1 & \alpha_1 & 0 & 0 & \cdots & 0 \\
-\beta_1 & I_2 & \alpha_2 & 0 & \cdots & 0 \\
0 & -\beta_2 & I_3 & \alpha_3 & \cdots & 0 \\
0 & 0 & -\beta_3 & I_4 & \cdots & 0 \\
0 & 0 & 0 & 0 & \cdots & -\beta_{N-1} \\
0 & 0 & 0 & 0 & \cdots & I_N
\end{vmatrix}
\]

Faldt, Petersson (1986)