Thermodynamics near the first order phase transition point of SU(3) gauge theory



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NFQCD 2018, YITP, Kyoto, June 8, 2018

### Phase structure of QCD at high temperature & density

- Phase transition lines
- Critical point
- First order transition at high density

Lattice QCD Simulations

 Direct simulation: Impossible at μ≠0.



### Quark Mass dependence of QCD phase transition



- The determination of the boundary of 1<sup>st</sup> order region: important.
- On the line of physical mass, the crossover at low density

→ 1<sup>st</sup> order transition at high density.

# Contents of this talk

- First order phase transition in the SU(3) gauge theory (Quenched QCD) and heavy quark region of QCD
- Domain wall between two phases at 1<sup>st</sup> order transition
- Latent heat and pressure gap
  - Derivative method
  - Gradient flow method
- Endpoint of the 1<sup>st</sup> order phase transition at finite quark mass and chemical potential.

# Distribution function & the effective potential $W(X;m,T,\mu) \equiv \frac{1}{Z} \int DU \delta(X - \hat{X}) (\det M(m,\mu))^{N_{\rm f}} e^{-S_g}$ (Histogram)

X: order parameters, total quark number, average plaquette, etc.



# Histogram method (Reweighting method)

Monte-Carlo method

- (Sg: gauge action, M: qaurk matrix)
- Generate configurations with the probability of the Boltzmann weight.

$$\langle O \rangle_{(m,T,\mu)} = \frac{1}{Z} \int DU O \left( \det M(m,\mu) \right)^{N_{\rm f}} e^{-S_g} \approx \frac{1}{N_{\rm conf.}} \sum_{\{\text{conf.}\}} O$$

• Distribution function (Histogram)

*X*: <u>order parameters</u>, <u>total quark number</u>, <u>average plaquette</u> etc.

$$W(X;m,T,\mu) = \frac{1}{Z} \int DU \,\delta(X-\hat{X}) (\det M(m,\mu))^{N_{\rm f}} e^{-S_g}$$
$$W(X) \approx \frac{1}{N_{\rm conf.}} \sum_{\{\text{conf.}\}} \delta(X-\hat{X}) \qquad \delta(\hat{X}) \approx \int_{\hat{X}}^{\text{Gauss}} \text{or} \qquad \hat{X}$$

• Expectation values

$$\langle O[X] \rangle_{(m,T,\mu)} = \frac{1}{Z} \int dX \ O[X] W(X,m,T,\mu), \ Z(m,T,\mu) = \int dX \ W(X,m,T,\mu)$$

Reweighting method for the plaquette distribution function

$$W(P,\beta,m,\mu) \equiv \int DU\delta(\hat{P}-P) \prod_{f=1}^{N_{\rm f}} \det M(m_f,\mu_f) e^{6N_{\rm site}\beta\hat{P}} \qquad (\beta = 6/g^2)$$

 $S_g = -6N_{\rm site}\beta\hat{P}$  plaquette *P* (1x1 Wilson loop for the standard action)

$$R(P,\beta,\beta_0m,m_0,\mu) \equiv W(P,\beta,m,\mu)/W(P,\beta_0,m_0,0) \qquad \text{(Reweight factor)}$$

$$R(P) = \frac{\left\langle \delta(\hat{P} - P) e^{6N_{\text{site}}(\beta - \beta_0)\hat{P}} \prod_{f} \frac{\det M(m_f, \mu_f)}{\det M(m_0, 0)} \right\rangle_{(\beta_0, \mu = 0)}}{\left\langle \delta(\hat{P} - P) \right\rangle_{(\beta_0, \mu = 0)}} \equiv \left\langle e^{6N_{\text{site}}(\beta - \beta_0)\hat{P}} \prod_{f} \frac{\det M(m_f, \mu_f)}{\det M(m_0, 0)} \right\rangle_{P:\text{fixed}}$$

Effective potential:

$$V_{\rm eff}\left(P,\beta,m,\mu\right) = -\ln\left[W\left(P,\beta,m,\mu\right)\right] = V_{\rm eff}\left(P,\beta_0,m_0,0\right) - \ln R\left(P,\beta,\beta_0,m,m_0,\mu\right)$$

## Distribution function in quenched simulations

Plaquette histogram at  $K=1/m_q=0$ .

dV eff/dP = 0 at the peak position of Veff (P).

In this case, the curvature of V<sub>eff</sub> is independent of  $\beta$ .

Derivative of *V*eff at  $\beta$ =5.69



First order phase transition

 $N_{\rm site} = 24^3 \times 4$ 

### Distribution function in a quenched simulation Derivative of the plaquette effective potential



## Histogram and Time history



- Polyakov loop: order parameter of the confinement
- Two peaks in the histogram.
- Flip-flops between two phases.
- Mixed configurations are rare.

## Two phases coexists at the 1<sup>st</sup> order PT

• Order parameter: Polyakov loop  $\Omega$  (spatial average)



 $\Omega = \frac{V_{\text{Cold}}\Omega_{\text{Cold}} + V_{\text{Hot}}\Omega_{\text{Hot}}}{V_{\text{Hot}}\Omega_{\text{Hot}}}$ 

If no energy loss at the phase boundary,  $V_{\rm eff}$  must be flat.



V: Volume

## Two phases coexists at the 1<sup>st</sup> order PT

• Order parameter: Polyakov loop  $\Omega$  (spatial average)



$$\Omega = \frac{V_{\text{Cold}}\Omega_{\text{Cold}} + V_{\text{Hot}}\Omega_{\text{Hot}}}{V}$$

The energy loss  $\Delta V$  at the phase boundary is in proportion to  $V^{2/3}$ 



$$\Delta F(\Omega) = \frac{\Delta V_{\rm eff}(\Omega)}{V} \sim \frac{1}{V^{1/3}}$$

## Energy loss at the domain wall



 $32^3 \times 8$  lattice  $48^3 \times 8$  lattice  $64^3 \times 8$  lattice

- $\Delta F(\Omega)$  is in proportion to  $1/V^{1/3}$ .
- It suggests a domain wall between two phases exsists at the 1<sup>st</sup> order phase transition.

## Latent heat and pressure gap Whot-QCD, Phys. Rev. D94, 014506 (2016) + $\alpha$

- The latent heat (energy gap) the most basic quantity.
- The gap of pressure must vanish. Reliability of the calculation can be confirmed.



- Gaps of energy density and pressure are measured using the derivative method.
  - Continuum extrapolation is performed.
- We tested the gradient flow method for the calculation of EoS.

[H. Suzuki, 2013]

balanced

### Thermodynamic quantities by the derivative method

$$[F. Karsch, Nucl. Phys. B205 (1982) 285]$$
anisotropic lattice
$$a_{s}$$
anisotropic la

Determination of the anisotropy coefficients at  $\xi = a_s/a_t = 1$ 

Isotropic lattice 
$$(\beta = \beta_s = \beta_t)$$
:  $\left(a_t \frac{\partial \beta_s}{\partial a_t}\right)_{\xi=1} = \left(a_t \frac{\partial \beta_t}{\partial a_t}\right)_{\xi=1} = a \frac{d\beta}{da_t}$ 



Data: Francis, kaczmarek, Laine, Neuhaus, Ohno, Phys. Rev. D 91, 096002 (2015) and our data for  $N_t = 4 \sim 22$ 

### String tension is independent of $\xi = \frac{a_s}{a_s}$

$$\left(\frac{\partial\beta_s}{\partial\xi} + \frac{\partial\beta_t}{\partial\xi}\right)_{a_t:\mathbf{fixed},\xi=1} = \frac{3}{2}a\frac{d\beta}{da}$$

[F. Karsch, Nucl. Phys. B205 (1982) 285]

### Ratio of the anisotropy coefficients

The slope of the phase transition line in the  $(\beta_s, \beta_t)$  plane:  $r_t$ 

[Ejiri, Iwasaki, Kanaya, Phys.Rev.D 58,094505 (1998)]

The slope of the transition line

Along the phase transition line,  $a_t$  is constant

because  $\frac{1}{T_c} = N_t a_t$ .

When one changes

$$(\beta_s, \beta_t) \rightarrow (\beta_s + d\beta_s, \beta_t + d\beta_t),$$

$$\mathrm{d}a_t = \frac{\partial a_t}{\partial \beta_t} d\beta_s + \frac{\partial a_t}{\partial \beta_t} d\beta_t = 0$$



$$\begin{pmatrix} \frac{\partial \beta_t}{\partial \beta_s} & \left(\frac{\partial \alpha_t}{\partial \beta_s}\right)_{\xi=1} & \left(\frac{\partial \beta_t}{\partial \xi}\right)_{\xi=1} \\ \begin{pmatrix} \frac{\partial \beta_s}{\partial a_t} & \frac{\partial \beta_t}{\partial a_t} \\ \frac{\partial \beta_s}{\partial \xi} & \frac{\partial \beta_t}{\partial \xi} \end{pmatrix} = \frac{1}{\left(\frac{\partial \xi}{\partial \beta_t}\right)\left(\frac{\partial a_t}{\partial \beta_s}\right) - \left(\frac{\partial \xi}{\partial \beta_s}\right)\left(\frac{\partial a_s}{\partial \beta_t}\right)} \begin{pmatrix} \frac{\partial \xi}{\partial \beta_t} & -\frac{\partial \xi}{\partial \beta_s} \\ -\frac{\partial a_t}{\partial \beta_t} & \frac{\partial a_t}{\partial \beta_s} \end{pmatrix}$$

 $r_{t} = \frac{d\beta_{s}}{d\beta_{s}} = -\frac{\left(\frac{\partial a_{t}}{\partial \beta_{t}}\right)_{\xi=1}}{d\beta_{t}} = \frac{\left(\frac{\partial \beta_{s}}{\partial \xi}\right)_{\xi=1}}{d\xi}$ 

#### Using the reweighting method, $(\beta_s, \beta_t)$ -dependence of the Polyakov loop susceptibility is measured.

### Anisotropy coefficients



Conventional combinations of the energy density and pressure

$$\frac{\Delta(\epsilon+p)}{T^4} = 3N_t^4 a \frac{d\beta}{da} \frac{r_t - 1}{r_t + 1} \{ (\langle P_s \rangle_{hot} - \langle P_s \rangle_{cold}) - (\langle P_t \rangle_{hot} - \langle P_t \rangle_{cold}) \}$$
$$\frac{\Delta(\epsilon-3p)}{T^4} = 3N_t^4 a \frac{d\beta}{da} \{ (\langle P_s \rangle_{hot} - \langle P_s \rangle_{cold}) - (\langle P_t \rangle_{hot} - \langle P_t \rangle_{cold}) \}$$

### Measurement of the slope of the transition line $r_t$



We used the reweighting method. The slope  $r_t$  can be determined with sufficient accuracy.

Order parameter: Polyakov loop  $\Omega(x, t)$ 

#### Transition point:

Peak position of Polyakov loop susceptibility





5.893 5.8935 5.894 5.8945 5.895 5.8955 5.896

 $\beta_t$ 

## Separation of the hot and cold phases



- We identify the phase by the Polyakov loop.
- Two peaks in the histogram.
- Flip-flops between two phases.
- Mixed configurations are rare. (We omit mixed configurations.)

### Vanishing pressure gap $\Delta p = 0$

$$\frac{\Delta p}{T^4} = N_t^4 \left\{ \frac{\partial \beta_s}{\partial \xi} \left( \langle P_s \rangle_{\text{hot}} - \langle P_s \rangle_{\text{cold}} \right) + \frac{\partial \beta_t}{\partial \xi} \left( \langle P_t \rangle_{\text{hot}} - \langle P_t \rangle_{\text{cold}} \right) \right\} = 0$$

Condition for  $\Delta p = 0$  $\frac{\partial \beta_s}{\partial \xi} = r_t = -\frac{\langle P_t \rangle_{hot} - \langle P_t \rangle_{cold}}{\langle P_s \rangle_{hot} - \langle P_s \rangle_{cold}}$ 

lattice	$r_t$	$\frac{\langle P_t \rangle_{hot} - \langle P_t \rangle_{cold}}{\langle P_s \rangle_{hot} - \langle P_s \rangle_{cold}}$
$48^{3} \times 6$	-1.2020(39)	1.216(50)
$64^3 \times 6$	-1.2022(52)	1.2053(38)
$48^3 \times 8$	-1.209(33)	1.204(14)
$64^3 \times 8$	-1.255(37)	1.2344(66)
$64^3 \times 12$	-1.16(61)	1.324(84)
$96^3 \times 12$	-1.204(53)	1.283(53)

The pressure gap is zero on each finite lattice.

### Continuum extrapolation of the latent heat

Fit the data at  $N_t = 6, 8, 12$  with a linear function of  $1/N_t^2$  assuming  $O(a^2)$  error.



Whot-QCD, Phys. Rev. D94, 014506 (2016)

## EoS by the Gradient Flow (H. Suzuki, 2013)

[H. Suzuki, Prog. Theor. Exp. Phys. 2014, 083B03 (2013); FlowQCD, Phys. Rev. D90, 011501(2014)]

- Gradient flow: smearing by a kind of diffusion equation
- Smeared field strength:  $F_{\mu\nu} \longrightarrow G_{\mu\nu} G_{\mu\nu}$
- Dim. 4 operators:  $E(t,x) = \frac{1}{4} \delta_{\mu\nu} G_{\rho\sigma}(t,x) G_{\rho\sigma}(t,x)$  $U_{\mu\nu}(t,x) = G_{\mu\rho}(t,x) G_{\nu\rho}(t,x) - \frac{1}{4} \delta_{\mu\nu} G_{\rho\sigma}(t,x) G_{\rho\sigma}(t,x)$
- Energy momentum tensor

$$T^{R}_{\mu\nu} = \lim_{t \to 0} \left\{ \frac{1}{\alpha_{U}(t)} U_{\mu\nu}(t,x) + \frac{\delta_{\mu\nu}}{4\alpha_{E}(t)} [E(t,x) - \langle E(t,x) \rangle_{0}] \right\}$$
$$\alpha_{U}(t) = g^{2} [1 + 2b_{0}s_{1}g^{2} + \cdots] \quad \alpha_{E}(t) = \frac{1}{2b_{0}} [1 + 2b_{0}s_{2}g^{2} + \cdots]$$

g: running coupling constant with  $\overline{MS}$  scheme based on the 4-loop beta function.

#### EOS by the Gradient Flow (H. Suzuki, 2013) [H. Suzuki, Prog. Theor. Exp. Phys. 2014, 083B03 (2013); FlowQCD, Phys. Rev. D90, 011501(2014)]

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• Energy density and Pressure

$$\epsilon = \langle T_{00} \rangle$$
  $p = \frac{1}{3} \sum_{i} \langle T_{ii} \rangle$ 

- Take the continuum limit for fixed flow time and volume
- Take the t=0 limit to remove unwanted higher dimension operators.
- Take the volume infinity limit



 $(N_s/N_t = V^{\overline{3}}T_c)$ 

- Lattice discretization error is reduced as t increases.
- Statistical error is also reduced.
- Continuum extrapolation form the data on the same volume

### Continuum extrapolation



• Continuum extrapolation for  $N_s/N_t = V^{\frac{1}{3}}T_c = 8$ .  $tT_c^2=0.013$ • Horizontal axis is  $1/N_t^2 \propto a_t^2$ .

## T-dependence, Continuum limit



- The same spatial volume  $(N_s/N_t = V^{\frac{1}{3}}T_c)$
- •We take the t=0 limit with t>0.008.
- magenta: continuum limit





- These two results are consistent within the errors.
- This results suggests  $\Delta p \rightarrow 0$ .



- These two results are consistent within the errors.
- This results suggests  $\Delta p \rightarrow 0$ .



- t=0 limit with keeping finite lattice spacing.  $\Delta p$ =0 for Nt=12 and 16.
- Continuum limit after t=0 limit and t=0 after continuum limit are consistent.

## Volume dependence of latent heat



Results by the derivative method

- The volume dependence is visible.
- The results by the gradient flow method approaches that by the derivative method as the volume increases.

 $N_{t} = 8$   $N_{t} = 12$   $N_{t} = 16$   $\Delta(\epsilon-3p)/T^{4}: derivative$   $\Delta\epsilon/T^{4}: derivative$ 

#### Endpoint of the first order Phase Transition (WHOT-QCD Collab., Phys.Rev.D84, 054502(2011); Phys.Rev.D89, 034507(2014))



- We study the properties of *W*(*X*) in the heavy quark region.
- Performing quenched simulations + Reweighting.
- We find the critical surface.
- Standard Wilson quark action + plaquette gauge action,  $S_g = -6N_{site}\beta P$

Hopping parameter expansion  $\kappa \sim 1/(\text{quark mass})$  $N_{\rm f} \ln \left( \frac{\det M(\kappa,\mu)}{\det M(0,0)} \right) = N_{\rm f} \left( 288N_{\rm site} \kappa^4 P + 12 \cdot 2^{N_t} N_s^3 \kappa^{N_t} \left( \cosh(\mu/T) \Omega_R + i \sinh(\mu/T) \Omega_I \right) + \cdots \right)$ phase

*P*: plaquette,  $\Omega = \Omega R + i \Omega I$ : Polyakov loop

det M(0,0) = 1

### Order of the phase transition Polyakov loop distribution (2-flavor)



 The pseudo-critical line is determined by χ<sub>Ω</sub> peak.



- Double-well at small  $\kappa$ 
  - First order transition
- Single-well at large  $\kappa$ 
  - Crossover

 $\kappa \sim 1/(quark mass)$ 

Phys.Rev.D89, 034507(2014)

#### Polyakov loop distribution in the complex plane $(2-flavor, \mu=0)$







 $\kappa^4 = 1.0 \times 10^{-5}$ 

 $\kappa^4 = 1.5 \times 10^{-5}$ 

1000



 $\kappa^4 = 2.0 \times 10^{-5}$ 





critical point

at  $\beta_{pc}$  measured by the Polyakov loop susceptibility.

# Determination of Critical K

• Effective potential on 32<sup>3</sup>x4 lattice



- The result on 24<sup>3</sup>x4 lattice is Kct=0.658(3)(<sup>+4</sup><sub>-11</sub>)
- No spatial volume dependence.

[Phys.Rev.D84, 054502(2011)]

## Determination of Critical K

• Effective potential on 48<sup>3</sup>x6 lattice



$$K_{ct,6} = 0.1021(11)$$

Meson mass at the critical point (2-flavor)  $m_{PS}$  : Pseudo scalar meson mass (T=0)

Two method

Reweighting using the detM by the hopping parameter expansion.
 Full QCD simulations (T=0) at the critical point.

	$N_{t}$	K <sub>cp</sub>	m <sub>PS</sub> a	$m_{\rm PS}/T_{\rm c}$
Reweighting	4	0.0641(18)	3.9332(24)	15.73(25)
	6	0.1021(11)	2.5048(23)	15.02(23)
full QCD	4	0.0641(18)	3.9354(22)	15.74(25)
	6	0.1021(11)	2.5059(15)	15.03(23)

- The results by the two methods are consistent.
- Nt (lattice spacing) dependence in  $m_{PS}/T_c$  is small.

### Critical surface in the heavy quark region of (2+1)-flavor QCD [Phys.Rev.D84, 054502(2011); Phys.Rev.D89, 034507(2014)] $(24^3 \times 4 \text{ lattice})$



## Summary

- We studied the first order phase transition in the SU(3) gauge theory (Quenched QCD) and heavy quark region of QCD
- The simulation results suggest that two phases are separated by a domain wall at 1<sup>st</sup> order transition.
- We measured the latent heat and pressure gap by the derivative method and gradient flow method.
- The pressure gap vanishes at the transition point.
- The endpoint of the 1<sup>st</sup> order phase transition at finite quark mass and chemical potential are measured.
- The spatial volume dependence and lattice spacing dependence in the location of the endpoint seems to be small.