KEK Lunch Seminar, 2023/09/29, KEK

1()

0.5

0.0

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_1.0

-1.5

-2.0

1.2

Thermodynamics of SU(3) Yang-Mills theory with boundary conditions

Masakiyo Kitazawa (YITP)

MK, Mogliacci, Kolbe, Horowitz, Phys. Rev. **D99** (2019) 094507 Suenaga, MK, Phys. Rev. **D107** (2023) 074502 D. Fujii, A. Iwanaka, D. Suenaga, MK, in prep.

Boundary Conditions in QFT

Many motivations

Casimir effect

Relativistic heavy-ion collisions

- Numerical simulations (ex. lattice QCD)
- Matsubara formalism for thermal systems





 \overline{T}



Matsubara Formalism

Thermal Field Theory

PBC for imaginary-time for bosons



 $T^{44} = -\epsilon$ $T^{11} = T^{22} = T^{33} = p$



Purpose

Thermal SU(3) YM with PBC along x direction



QFT on $T^2 \times R^2$

How does thermodynamics behave w.r.t. T and L_{χ} ?

Thermal Casimir effect in a non-perturbative system
 QCD phase diagram as a function of L_x
 2 Polyakov loops will play important roles

Contents

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MK+, Phys. Rev. **D99** (2019) 094507

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attractive force between two conductive plates

Brown, Maclay 1969



x z y

Brown, Maclay 1969



Brown, Maclay 1969



Pressure Anisotropy (a) $T \neq 0$



Pressure Anisotropy (a) $T \neq 0$



MK, Mogliacci, Kolbe, Horowitz, in prep.

Free scalar field $\Box L_2 = L_3 = \infty$ \Box Periodic BC Mogliacci+, 1807.07871

Lattice result

Periodic BC
Only t→0 limit
Error: stat.+sys.

Medium near T_c is remarkably insensitive to finite size!

Thermodynamics on the Lattice

Various Methods

□ Integral, differential, moving frame, non-equilibrium, ... □ rely on thermodynamic relations valid in V→∞ $P = \frac{T}{V} \ln Z$ $sT = \varepsilon + P$ Not applicable to anisotropic systems

UWe employ **Gradient Flow Method** $\varepsilon = \langle T_{00} \rangle$ $P = \langle T_{11} \rangle$ **Components of EMT are directly accessible!**

Yang-Mills Gradient Flow



□ diffusion equation in 4-dim space
 □ diffusion distance d ~ √8t
 □ "continuous" cooling/smearing
 □ No UV divergence at t>0



Small Flow-Time Expansion

Luescher, Weisz, 2011 Suzuki, 2013

 $\tilde{\mathcal{O}}(t,x) \xrightarrow[t \to 0]{} \sum_{i \to 0} \sum_{i} c_i(t) \mathcal{O}_i^R(x)$

an operator at t>0

 $\tilde{\mathcal{O}}(t,x)$

t→0 limit

remormalized operators of original theory



Constructing EMT

Suzuki, 2013

$$U_{\mu\nu}(t,x) = \alpha_U(t) \left[T^R_{\mu\nu}(x) - \frac{1}{4} \delta_{\mu\nu} T^R_{\rho\rho}(x) \right] + \mathcal{O}(t)$$
$$E(t,x) = \langle E(t,x) \rangle + \alpha_E(t) T^R_{\rho\rho}(x) + \mathcal{O}(t)$$
vacuum subtr.



Remormalized EMT

$$T^{R}_{\mu\nu}(x) = \lim_{t \to 0} \left[c_1(t) U_{\mu\nu}(t, x) + \delta_{\mu\nu} c_2(t) E(t, x)_{\text{subt.}} \right]$$

Perturbative coefficient: Suzuki (2013); Makino, Suzuki (2014); Harlander+ (2018); Iritani, MK, Suzuki, Takaura (2019)

Thermodynamics



Systematic error: μ_0 or μ_d , Λ , t $\rightarrow 0$ function, fit range

Good agreement between different methods
 Our method can investigate finite systems with BCs

Numerical Setup

SU(3) YM theoryWilson gauge action

N_t = 16, 12
N_z/N_t=6
2000~4000 confs.
Even N_x

No Continuum extrap.

Same Spatial volume

- 12X72²X12 ~ 16X96²X16
- 18x72²x12 ~ 24x96²x16

T/T_c	β	N_z	$N_{ au}$	N_x	$N_{\rm vac}$
1.12	6.418	72	12	12, 14, 16, 18	64
	6.631	96	16	16, 18, 20, 22, 24	- 96
1.40	6.582	72	12	12, 14, 16, 18	64
	6.800	96	16	16, 18, 20, 22, 24	128
1.68	6.719	72	12	12, 14, 16, 18, 24	64
	6.719	96	12	14, 18	64
	6.941	96	16	16, 18, 20, 22, 24	- 96
2.10	6.891	72	12	12, 14, 16, 18, 24	72
	7.117	96	16	16, 18, 20, 22, 24	128
2.69	7.086	72	12	12, 14, 16, 18	-
$\simeq 8.1$	8.0	72	12	12, 14, 16, 18	-
$\simeq 25$	9.0	72	12	12, 14, 16, 18	-

Simulations on OCTOPUS/Reedbush

Pressure Anisotropy (a) $T \neq 0$



MK, Mogliacci, Kolbe, Horowitz, in prep.

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HigherT

High-T limit: massless free gluons How does the anisotropy approach this limit?

Difficulties

□ Vacuum subtraction requires large-volume simulations. □ Lattice spacing not available $\rightarrow c_1(t), c_2(t)$ are not determined.

HigherT

High-T limit: massless free gluons How does the anisotropy approach this limit?

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We study

$$rac{x+\delta}{z+\delta}$$
 δ =

$$\delta = -\frac{1}{4} \sum_{\mu} T^{\rm E}_{\mu\mu}$$

No vacuum subtr. nor Suzuki coeffs. necessary!

 $\frac{P_x + \delta}{P_z + \delta}$



 $T/Tc \cong 8.1 \ (b = 8.0) \ / \ T/Tc \cong 25 \ (b = 9.0)$

Ratio approaches the asymptotic value for large T.
 But, large deviation exists even at T/Tc~25.
 1st-order phase transition??

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Thermodynamics of SU(3) YM on $S^1 \times R^3$



□ Deconfinement phase transition = 1st-order PT
 □ Stefen-Boltzmann limit for T → ∞
 → How to describe these features quantitatively?

Polyakov-loop Effective Models

Meisinger+, PRD (2003)

General Idea

Introduce Polyakov loop P through a constant background field A₀

$$P = \operatorname{Tr} \left[\mathcal{P} \exp \left(i \int_{0}^{L_{\tau}} A_{\tau} d\tau \right) \right] \quad \checkmark \quad A_{\tau}(x) = \begin{pmatrix} \theta_{1} & 0 & 0 \\ 0 & \theta_{2} & 0 \\ 0 & 0 & \theta_{3} \end{pmatrix}$$

Note: $\square P = 0$: confinement / Z(3) symmetric $\square P \neq 0$: deconfinement / Z(3) broken

Polyakov-loop Effective Models

Meisinger+, PRD (2003)

Free Energy $F(T; P) = F_{\text{pert.}}(T; P) + F_{\text{pot.}}(T; P)$

Perturbative term

free energy of massless free gluons with a constant A_{τ}

$$f_{pert}(\theta) = \sum_{n \in \mathbb{Z}} \int \frac{d^3k}{(2\pi)^3} \operatorname{tr}_A \ln \left[\left(\frac{2\pi n}{\beta} - A_0 \right)^2 + \vec{k}^2 \right]$$

Polyakov-loop potential Phenomenological free energy that makes *P* nontrivial

The value of P is determined so as to minimize F(T; P).

 $F_{\rm pot}(T,P)$

Meisinger+, PRD (2003)

DModel A

gluon mass term at the leading order

$$F_{\rm gluons} = F_{\rm pert} + m_g^2 \tilde{F} + \cdots$$

employ this term as F_{pot} with a parameter m_g

□Model B

term inspired by the Haar measure

$$F_{\text{pot}} = -\frac{T}{R^3} \ln \prod_{j < k} \sin^2 \left(\frac{\theta_j - \theta_k}{2}\right)$$

R: phenomenological parameter

Results

Meisinger+, PRD ('03)

Dumitru+, PRD ('12)



Qualitative behavior of lattice thermodynamics near and above T_c is well explained.

Extension to $T^2 \times R^2$

Suenaga, MK ('23); Fujii+, in prep.

2 Polyakov loops along au and x directions

$$P_{\tau} = \operatorname{Tr}\left[\mathcal{P}\exp\left(i\int_{0}^{L_{\tau}}A_{\tau}d\tau\right)\right] \qquad P_{x} = \operatorname{Tr}\left[\mathcal{P}\exp\left(i\int_{0}^{L_{\tau}}A_{x}d\tau\right)\right]$$

Diagonal ansatz: $A_i = \begin{pmatrix} \theta_1 & 0 & 0 \\ 0 & \theta_2 & 0 \\ 0 & 0 & \theta_3 \end{pmatrix}$

$$F_{\text{pert.}} = F_{\text{pert}}(L_{\tau}, L_{x}; \vec{\theta}_{\tau}, \vec{\theta}_{x})$$
$$F_{\text{pot.}} = F_{\text{pot}}(L_{\tau}, L_{x}; \vec{\theta}_{\tau}, \vec{\theta}_{x})$$

Constraints on F_{pot}



Invariance w.r.t. exchange of τ , xaxes $F(\vec{\theta_{\tau}}, \vec{\theta_{x}}; L_{\tau}, L_{x}) = F(\vec{\theta_{x}}, \vec{\theta_{\tau}}; L_{x}, L_{\tau})$ Thermodynamics on $S^{1} \times R^{3}$

must be reproduced at $L_x \rightarrow \infty$

 $F_{\text{pert}}(L_{\tau}, L_x) \xrightarrow[L_x \to \infty]{} \mathcal{O}(L_x^{-3})$

 $F_{\rm pot}(L_{ au}, L_x)$ must disappear faster

Separable Ansatz

Suenaga, MK ('23)

$$F_{\text{pot}} = F_{\text{pot}}^{S^1 \times R^3} (L_{\tau}; \vec{\theta}_{\tau}) + F_{\text{pot}}^{S^1 \times R^3} (L_x; \vec{\theta}_x)$$



Lattice result is not reproduced even qualitatively.

Phase Diagram



Introducing Cross Term Fujii+, in prep.

Free Energy $F = F_{\text{pert.}} + F_{\text{pot}} + F_{\text{cross}}$

cross term of P_{τ} and P_{χ}

 $F_{\text{cross}} = g(L_{\tau}, L_{x}) \left[c_{4} \text{Tr}[P_{\tau}^{\dagger}P_{\tau}] \text{Tr}[P_{x}^{\dagger}P_{x}] + c_{5} (\text{Tr}[P_{\tau}^{\dagger}P_{\tau}] \text{Tr}[P_{x}^{3}] + \text{Tr}[P_{\tau}^{3}] \text{Tr}[P_{x}^{\dagger}P_{x}]) + c_{6} \text{Tr}[P_{\tau}^{3}] \text{Tr}[P_{x}^{3}] \right]$

 c_4, c_5, c_6 : parameters in the model

$\begin{aligned} & \left[F_{\text{cross}} = g(L_{\tau}, L_{x}) \left[c_{4} \text{Tr}[P_{\tau}^{\dagger} P_{\tau}] \text{Tr}[P_{x}^{\dagger} P_{x}] \right. \\ & \left. + c_{5} (\text{Tr}[P_{\tau}^{\dagger} P_{\tau}] \text{Tr}[P_{x}^{3}] + \text{Tr}[P_{\tau}^{3}] \text{Tr}[P_{x}^{\dagger} P_{x}] \right) \right. \\ & \left. + c_{6} \text{Tr}[P_{\tau}^{3}] \text{Tr}[P_{x}^{3}] \right] \end{aligned}$



 $g(L_{\tau}, L_{x}) = T_{c}^{4} \left((T_{c}L_{\tau})^{2} + (T_{c}L_{x})^{2} \right)^{-n}$ 1.5 < n < 2.0

 $F_{\text{pot}}^{S^1 \times \overline{R^3}} \xrightarrow[L_{\tau}, L_x \to 0]{} \mathcal{O}(L_c^{-2})$ $F_{\text{pert}} \xrightarrow[L_c \to \infty]{} \mathcal{O}(L_c^{-3})$

Result

 $T/T_c = 1.68$



Lattice results for T/T_c > 1.5 are well reproduced.
 No parameters to fit the results for T/T_c = 1.4, 1.12.
 Appearance of 1st-order PT?

Phase Diagram



 Appearance of a new 1st PT and critical points in the confined region
 How do it affect lattice simulations?



Polyakov Loops



Competition between P_{τ} and P_{χ} leads to their sudden changes around $L_{\tau} \simeq L_{\chi}$.

Thermodynamics







n Dependence



The value of *n* can be constrained by the high-T behavior.

Summary

Lattice thermodynamics in SU(3) YM with periodic BC¹⁶ have peculiar behaviors:

 $T/T_{c} = 2.10$

1.8

- Medium at 1.4<T/T_c<2.1 is remarkably insensitive to the boundary.</p>
- \Box Slow approach to the SB limit at small L_{τ} , L_{χ} .

Our model with two Polyakov loops explains the lattice results for $T \ge 1.5T_c$ qualitatively: Interplay b/w two Polyakov loops plays a crucial role. Appearance of new 1st-PT & CP is predicted.

Future More lattice results Anti-periodic / Dirichlet BCs, BC for two directions, below T_c, ...





energy densty / transverse P

Energy Density

Transverse Pressure P_z





Gradient Flow Method



Take Extrapolation (t,a) \rightarrow (0,0) $\langle T_{\mu\nu}(t) \rangle_{\text{latt}} = \langle T_{\mu\nu}(t) \rangle_{\text{phys}} + \begin{bmatrix} C_{\mu\nu}t \\ D_{\mu\nu}t \\ t \end{bmatrix} + \begin{bmatrix} D_{\mu\nu}\frac{a^2}{t} \end{bmatrix} + \cdots$ O(t) terms in SFTE lattice discretization

Two Special Cases with PBC $1/T \ll L_x = L_y = L_z$ $1/T = L_x, \ L_y = L_z$ $\frac{1}{T}$ L_y, L_z $\overline{L}_y, \ \underline{L}_z$ L_x $T_{11} = T_{22} = T_{33}$ $T_{44} = T_{11}, \ T_{22} = T_{33}$ In conformal ($\Sigma_{\mu}T_{\mu\mu}=0$) $\underline{p_1}$ - 1 $\frac{p_1}{-} = -1$ p_2 p_2

EMT on the Lattice: Conventional

 $\begin{aligned} & \text{Lattice EMT Operator}_{\text{Caracciolo+, 1990}} \\ & T_{\mu\nu} = Z_6 T_{\mu\nu}^{[6]} + Z_3 T_{\mu\nu}^{[3]} + Z_1 \left(T_{\mu\nu}^{[1]} - \left\langle T_{\mu\nu}^{[1]} \right\rangle \right) \\ & T_{\mu\nu}^{[6]} = (1 - \delta_{\mu\nu}) F_{\mu\rho}^a F_{\nu\rho}^a, \ T_{\mu\nu}^{[3]} = \delta_{\mu\nu} \left(F_{\mu\rho}^a F_{\nu\rho}^a - \frac{1}{4} F_{\rho\sigma}^a F_{\rho\sigma}^a \right), \ T_{\mu\nu}^{[1]} = \delta_{\mu\nu} F_{\rho\sigma}^a F_{\rho\sigma}^a \end{aligned}$

\Box Fit to thermodynamics: Z_3, Z_1

Shifted-boundary method: Z₆, Z₃ Giusti, Meyer, 2011; 2013; Giusti, Pepe, 2014~; Borsanyi+, 2018

Multi-level algorithm

effective in reducing statistical error of correlator

Meyer, 2007; Borsanyi, 2018; Astrakhantsev+, 2018

Perturbative Coefficients



Choice of the scale of g²

 $c_1(t) = c_1\left(g^2(\mu(t))\right)$

Previous: $\mu_d(t) = 1/\sqrt{8t}$ Improved: $\mu_0(t) = 1/\sqrt{2e^{\gamma_E}t}$

Harlander+ (2018)



Iritani, MK, Suzuki, Takaura, PTEP 2019

I dependence becomes milder with higher order coeff.
 Better t→o extrapolation

Systematic error: μ_0 or μ_d , uncertainty of Λ (±3%), fit range Extrapolation func: linear, higher order term in c_1 (~g⁶)

Small-t Extrapolation $T/T_c = 1.68$



•
$$P_x$$
, • P_z , $L_1T = 3/2$
• P_x , • P_z , $L_1T = 9/8$
• P_x , • P_z , $L_1T = 1$

Filled: N_t=16 / Open: N_t=12

Small-t extrapolation

- Solid: N_t=16, Range-1
- Dotted: N_t=16, Range-2,3
- Dashed: N_t=12, Range-1

□ Stable small-t extrapolation □ No N_t dependence within statistics for $L_xT=1$, 1.5

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•
$$P_x$$
, • P_z , $L_1T = 3/2$
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