Thermodynamic Potential of the Polyakov Loop in SU(3) Quenched Lattice QCD

H. Suganuma (Kyoto U.)

in collaboration with H. Ohata, M. Kitazawa (YITP, Kyoto U.)

Abstract:

Using SU(3) lattice QCD, we study the effective potential (thermodynamic potential) of the Polyakov loop at finite temperature in the field theoretical manner for the first time. We adopt SU(3) quenched QCD on a spatially large lattice of $64^3 \times 6$ at $\beta = 5.89379$, just corresponding to the critical temperature T_c of the deconfinement phase transition. From 200,000 gauge configurations, we numerically evaluate the effective potential using the reweighting method for the lattice QCD data around each vacuum of Z_3 -symmetric and Z_3 -broken vacua.

ICNFP2023, 21 July 2023, Zoom, OAC, Crete

Introduction : Confinement and Polyakov loop

Color Confinement and Chiral Symmetry Breaking are most important phenomena of Nonperturbative QCD. In particular, Confinement is a very curious phenomenon peculiar to QCD, and its understanding is still an extremely difficult problem.

Lattice QCD result for Inter-quark potential



Introduction : Confinement and Polyakov loop

In finite temperature QCD, a standard order parameter of quark confinement is the Polyakov loop $\langle P \rangle$, defined as a path-ordered product along imaginary time:

$$P \equiv \operatorname{tr} \operatorname{Pexp}\{i \int_0^{1/T} dt A_t(\mathbf{x}, t)\}, \quad \langle P \rangle \propto e^{-E_q/T}$$

The thermal expectation value of the Polyakov loop $\langle P \rangle$ is related to the single-quark free energy E_q .

In the confinement phase, the Polyakov loop $\langle P \rangle$ is (almost) zero, because the single-quark energy is infinite $E_q = \infty$, reflecting quark confinement.

In the deconfinement phase, the Polyakov loop $\langle P \rangle$ takes a finite value, and the single-quark energy E_q becomes finite.

Order parameter of Confinement: Polyakov loop $\langle P \rangle \propto e^{-E_q/T}$

Introduction : Polyakov loop and Z_{Nc} center symmetry

In the lattice QCD formalism,

the Polyakov loop is also an order parameter of Z_{Nc} center symmetry, which relates to the spatially global transformation of temporal link variables at a fixed time.

Under the Z_{Nc} transformation, the lattice gauge action is invariant, but the Polyakov loop *P* is variant and behaves as its order parameter.

- The confinement phase is Z_{Nc} -symmetric owing to $\langle P \rangle = 0$.
- In the deconfinement phase, Z_{Nc} center symmetry is spontaneously broken because of $\langle P \rangle \neq 0$.

Lattice QCD result of Polyakov Loop (P) at finite temperature

Scatter plot of Polyakov loop

 Z_3 -symmetric Confinement Phase

 Z_3 -broken Deconfinement Phase



M. Goeckeler et al. Nucl. Phys. B Proc. Suppl. 94 (2001) 402.

 Z_3 center symmetric structure and its spontaneous breaking at high temperature

In spite of importance of Polyakov loop $\langle P \rangle$ in QCD, its thermodynamic potential has not been calculated directly from QCD before our study.

Field-theoretical Formalism

Basically, we derive Effective Potential (thermodynamic potential) of Polyakov loop using standard field-theoretical manner based on lattice formalism.

For the Polyakov loop P defined on $L_s^3 \times L_t$ lattice

 $P(\vec{x}) \equiv \frac{1}{N_c} \operatorname{Tr}[U_4(1, \vec{x})U_4(2, \vec{x}) \cdots U_4(L_t, \vec{x})] = P_{\operatorname{Re}}(\vec{x}) + iP_{\operatorname{Im}}(\vec{x}) \in \mathbb{C}$

we prepare source J of Polyakov loop

$$J(\vec{x}) \equiv J_{\text{Re}}(\vec{x}) + iJ_{\text{Im}}(\vec{x}) \in \mathbf{C}$$

We define the QCD generating functional including the source *J* of the Polyakov loop:

$$Z[J] = \int DU \exp\{-S[U] + \operatorname{Re}(J \cdot P^{\dagger})\}$$
$$= \int DU \exp\{-S[U] + J_{\operatorname{Re}} \cdot P_{\operatorname{Re}} + J_{\operatorname{Im}} \cdot R_{\operatorname{Im}})\}$$

Here, the inner product denotes the spatial summation

$$J \cdot P^{\dagger} \equiv \frac{1}{L_s^3} \sum_{\vec{x}} J(\vec{x}) \cdot P^{\dagger}(\vec{x})$$
 etc

Field-theoretical Formalism

Generating functional W for connected diagrams is defined as usual.

$$W[J] \equiv \ln Z[J]$$

Physically, its derivative with respect to source J gives the expectation vale of Polyakov loop

$$\frac{\partial W[J_{\rm Re}, J_{\rm Im}]}{\partial J_{\rm Re}} = \frac{1}{Z[J]} \int DU e^{-S + J_{\rm Re} \cdot P_{\rm Re} + J_{\rm Im} \cdot P_{\rm Im}} P_{\rm Re} = \langle P_{\rm Re} \rangle_J$$

$$\frac{\partial W[J_{\rm Re}, J_{\rm Im}]}{\partial J_{\rm Im}} = \frac{1}{Z[J]} \int DU e^{-S + J_{\rm Re} \cdot P_{\rm Re} + J_{\rm Im} \cdot P_{\rm Im}} P_{\rm Im} = \langle P_{\rm Im} \rangle_J$$

Effective Potential of Polyakov loop is defined as its Legendre transformation in standard field-theoretical manner:

$$V_{\text{eff}}[\langle P \rangle] \equiv J_{\text{Re}} \langle P_{\text{Re}} \rangle_J + J_{\text{Im}} \langle P_{\text{Im}} \rangle_J - W[J] \Big|_{J(\langle P \rangle)}$$
$$P(\vec{x}) = P_{\text{Re}}(\vec{x}) + iP_{\text{Im}}(\vec{x}) \in \mathbf{C} \qquad J(\vec{x}) \equiv J_{\text{Re}}(\vec{x}) + iJ_{\text{Im}}(\vec{x}) \in \mathbf{C}$$

Effective Potential

(Thermodynamic Potential or Free Energy at finite temperature)

$$V_{\rm eff} \left[\left\langle P \right\rangle \right] = J_{\rm Re} \left\langle P_{\rm Re} \right\rangle_J + J_{\rm Im} \left\langle P_{\rm Im} \right\rangle_J - W[J] \Big|_{J(\left\langle P \right\rangle)}$$

 $P(\vec{x}) = P_{\text{Re}}(\vec{x}) + iP_{\text{Im}}(\vec{x}) \in \mathbb{C} \qquad J(\vec{x}) \equiv J_{\text{Re}}(\vec{x}) + iJ_{\text{Im}}(\vec{x}) \in \mathbb{C}$

At finite temperature, the *Effective Potential* physically means *Thermodynamic Potential or Free Energy* as function of Polyakov loop, and satisfies the following extremal condition:

$$\frac{\partial V_{\rm eff}[\langle P_{\rm Re} \rangle, \langle P_{\rm Im} \rangle]}{\partial \langle P_{\rm Re} \rangle} = J_{\rm Re}$$

$$\frac{\partial V_{\rm eff} [\langle P_{\rm Re} \rangle, \langle P_{\rm Im} \rangle]}{\partial \langle P_{\rm Im} \rangle} = J_{\rm Im}$$

Field-theoretical derivation of Effective Potential

$$V_{\text{eff}}\left[\left\langle P\right\rangle\right] = J_{\text{Re}}\left[\left\langle P_{\text{Re}}\right\rangle_{J} + J_{\text{Im}}\left\langle P_{\text{Im}}\right\rangle_{J} - \underline{W[J]}\right|_{J(\langle P \rangle)} \begin{vmatrix} P(\vec{x}) = P_{\text{Re}}(\vec{x}) + iP_{\text{Im}}(\vec{x}) \in \mathbf{C} \\ J(\vec{x}) \equiv J_{\text{Re}}(\vec{x}) + iJ_{\text{Im}}(\vec{x}) \in \mathbf{C} \end{vmatrix}$$

As for W[J], it can be expressed with expectation value without source (J = 0) apart form an irrelevant constant:

$$W[J] - W[0] = \ln \frac{Z[J]}{Z[0]} = \ln \frac{\int DU e^{-S[U] + J_{\text{Re}} \cdot P_{\text{Re}}[U] + J_{\text{Im}} \cdot P_{\text{Im}}[U]}}{\int DU e^{-S[U]}} = \ln \left\langle e^{J_{\text{Re}} \cdot P_{\text{Re}} + J_{\text{Im}} \cdot P_{\text{Im}}} \right\rangle_{J=0}$$

Polyakov loop $\langle P \rangle_J$ in the presence of source J can be also expressed with expectation value without source (J = 0):

$$\left\langle P_{\text{Re/Im}} \right\rangle_{J} = \frac{\int DU \, e^{-S[U] + J_{\text{Re}} \cdot P_{\text{Re}}[U] + J_{\text{Im}} \cdot P_{\text{Im}}[U]} P_{\text{Re/Im}}[U]}{\int DU \, e^{-S[U] + J_{\text{Re}} \cdot P_{\text{Re}}[U] + J_{\text{Im}} \cdot P_{\text{Im}}[U]}} = \frac{\left\langle e^{J_{\text{Re}} \cdot P_{\text{Re}} + J_{\text{Im}} \cdot P_{\text{Im}}} P_{\text{Re/Im}} \right\rangle_{J=0}}{\left\langle e^{J_{\text{Re}} \cdot P_{\text{Re}} + J_{\text{Im}} \cdot P_{\text{Im}}} \right\rangle_{J=0}}$$

In lattice QCD, physical quantities in the presence of source J can be calculated using expectation value without source (J = 0) by regarding the source factor $exp(J \cdot P)$ as an operator, which is called reweighting method.

Lattice QCD derivation of Effective Potential

In the practical calculation in lattice QCD, we use the following procedure. First, we numerically calculate the following expectation values without source (J = 0) using gauge configurations generated in lattice QCD:

$$\left\langle e^{J_{\mathrm{Re}} \cdot P_{\mathrm{Re}}[U] + J_{\mathrm{Im}} \cdot P_{\mathrm{Im}}[U]} \right\rangle_{J=0} = \frac{1}{N_{\mathrm{config}}} \sum_{n=1}^{N_{\mathrm{config}}} e^{J_{\mathrm{Re}} \cdot P_{\mathrm{Re}}[U_n] + J_{\mathrm{Im}} \cdot P_{\mathrm{Im}}[U_n]}$$

$$\left\langle e^{J_{\mathrm{Re}} \cdot P_{\mathrm{Re}} + J_{\mathrm{Im}} \cdot P_{\mathrm{Im}}} P_{\mathrm{Re}/\mathrm{Im}} \right\rangle_{J=0} = \frac{1}{N_{\mathrm{config}}} \sum_{n=1}^{N_{\mathrm{config}}} e^{J_{\mathrm{Re}} \cdot P_{\mathrm{Re}}[U_n] + J_{\mathrm{Im}} \cdot P_{\mathrm{Im}}[U_n]} P_{\mathrm{Re}/\mathrm{Im}}[U_n]$$

Second, we calculate W[J] and expectation values of Polyakov loop $\langle P \rangle_J$ in presence of source *J*, using these expectation values without source (*J* = 0):

$$W[J] - W[0] = \ln \frac{Z[J]}{Z[0]} = \ln \frac{\int DU \, e^{-S[U] + J_{\text{Re}} \cdot P_{\text{Re}}[U] + J_{\text{Im}} \cdot P_{\text{Im}}[U]}}{\int DU \, e^{-S[U]}} = \ln \left\langle e^{J_{\text{Re}} \cdot P_{\text{Re}} + J_{\text{Im}} \cdot P_{\text{Im}}} \right\rangle_{J=0}$$

$$\left\langle P_{\text{Re/Im}} \right\rangle_{J} = \frac{\int DU \, e^{-S[U] + J_{\text{Re}} \cdot P_{\text{Re}}[U] + J_{\text{Im}} \cdot P_{\text{Im}}[U]} P_{\text{Re/Im}}[U]}{\int DU \, e^{-S[U] + J_{\text{Re}} \cdot P_{\text{Re}}[U] + J_{\text{Im}} \cdot P_{\text{Im}}[U]}} = \frac{\left\langle e^{J_{\text{Re}} \cdot P_{\text{Re}} + J_{\text{Im}} \cdot P_{\text{Im}}} \right\rangle_{J=0}}{\left\langle e^{J_{\text{Re}} \cdot P_{\text{Re}} + J_{\text{Im}} \cdot P_{\text{Im}}} \right\rangle_{J=0}}$$

Thus, we obtain *Effective Potential of Polyakov loop* apart from an irrelevant constant.

$$V_{\rm eff}\left[\left\langle P\right\rangle\right] = J_{\rm Re}\left\langle P_{\rm Re}\right\rangle_J + J_{\rm Im}\left\langle P_{\rm Im}\right\rangle_J - \left(W[J] - W[0]\right) \begin{array}{c}P(\vec{x}) = P_{\rm Re}(\vec{x}) + iP_{\rm Im}(\vec{x}) \in \mathbf{C}\\J(\vec{x}) \equiv J_{\rm Re}(\vec{x}) + iJ_{\rm Im}(\vec{x}) \in \mathbf{C}\end{array}$$

Lattice QCD setup

We use SU(3) quenched QCD with standard plaquette action on a spatially large lattice of $64^3 \times 6$ at $\beta = 5.89379$, which corresponds to the critical temperature $T_c = 280$ MeV of the deconfinement phase transition in quenched QCD. The lattice spacing is about a = 0.12fm.

We use huge number of 200,000 gauge configurations generated with usual Monte Carlo method based on pseudo-heat bath algorithm.

In lattice QCD, each of generated configuration represents typical QCD vacuum, and therefore these gauge configurations give "ensemble of thermal QCD vacuum".

As for the Polyakov-loop source $J=(J_{Re}, J_{Im})$, we use 1001 different points. Lattice QCD result for Scatter Plot of Polyakov loop $\langle P \rangle_{J=0}$ Each point corresponds to the lattice gauge configuration.



Lattice QCD result for Scatter Plot of Polyakov loop $\langle P \rangle_{J=0}$ Each point corresponds to the lattice gauge configuration.



At Critical temperature *T_c*, Confined and Deconfined Vacua coexist. Caution: *Naïve Averaging* over all the data leads to *Nonsense Zero Expectation Value* !

Histogram of Polyakov loop $\langle P \rangle_{J=0}$ at Critical Temperature



Lattice QCD derivation of Effective Potential

Caution: In the case of Coexistence of Vacua, dangerous naïve averaging has to be avoided.

Therefore, as a technical improvement, around each vacuum of Z_3 -symmetric and Z_3 -broken vacua, we use the corresponding lattice QCD data for the reweighting method.

Procedure:

- 1. For each lattice gauge configuration, we calculate Polyakov loop $\langle P \rangle_{J=0}$.
- 2. For each lattice gauge configuration, we associate them with each vacuum among Z_3 -symmetric and Z_3 -broken vacua.
- Around each vacuum, using lattice QCD data associated to each vacuum, we numerically derive *Effective Potential V_{eff}[(P)] of Polyakov loop (P)* with the reweighting method.

1. Write Scatter Plot of Polyakov loop $\langle P \rangle_{J=0}$ for lattice gauge configurations.





3. Around each vacuum, using lattice QCD data associated to each vacuum, we numerically derive *Effective Potential* $V_{eff}[\langle P \rangle]$ with the reweighting method.







Summary and Conclusion

Using SU(3) lattice QCD, we have studied the effective potential (thermodynamic potential) of the Polyakov loop at finite temperature in the field theoretical manner for the first time.

We have adopted SU(3) quenched QCD on a spatially large lattice of $64^3 \times 6$ at $\beta = 5.89379$, corresponding to the critical temperature T_c of the deconfinement phase transition.

From 200,000 gauge configurations, we have numerically evaluated the effective potential using the reweighting method for the lattice QCD data around each vacuum of Z_3 -symmetric and Z_3 -broken vacua.

