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Letter

Entanglement in four-dimensional SU(3) gauge theory

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We investigate the quantum entanglement entropy for the four-dimensional Euclidean SU(3) gauge theory. We present the first non-perturbative calculation of the entropic c-function ($C(l)$) of SU(3) gauge theory in lattice Monte Carlo simulation using the replica method. For $0 \leqslant l \leqslant 0.7\,\mathrm{fm}$, where l is the length of the subspace, the entropic c-function is almost constant, indicating conformally invariant dynamics. The value of the constant agrees with that perturbatively obtained from free gluons, with 20% discrepancy. When l is close to the $\Lambda_{\mathrm{QCD}}^{-1}$ $\left(\sim T_c^{-1}\right)$ scale, the entropic c-function decreases smoothly, and it is consistent with zero within error bars at $l \gtrsim 0.9\,\mathrm{fm}$.

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Quantum entanglement is a fascinating phenomenon that was first highlighted by the Einstein–Podolsky–Rosen paradox [1] and has remained a focus of research activity for decades. If there is a system in a pure quantum state, measurements on a subsystem A determine the results of measurements on its complement B, even if no causal communication is possible between the two measurements. The entanglement entropy S_A of subsystem A is defined as von Neumann entropy corresponding to the reduced density matrix ρ_A:

$$S_A = -\mathrm{Tr}_{\mathcal{H}_A} \rho_A \log(\rho_A), \tag{1}$$

where $\rho_A = \mathrm{Tr}_{\mathcal{H}_B}[\rho_{\mathrm{tot}}]$, and it is assumed that the total Hilbert space is a direct product of two subspaces corresponding to the subsystems considered, $\mathcal{H}_{\mathrm{tot}} = \mathcal{H}_A \otimes \mathcal{H}_B$.

More generally, studies of entanglement entropy become central in cases of complex systems with strong interactions, where the properties of the ground state cannot be evaluated directly. In particular, the notion of quantum entanglement is crucial for the theory of quantum phase transitions, i.e., non-thermal phase transitions at temperature $T = 0$ [2–4]. In the physics of black holes, consideration of quantum entanglement is central to discussions of the information paradox [5,6], which challenges the consistency of general relativity and quantum mechanics.

Applications to field theory are more recent. First of all, the entanglement entropy is ultraviolet divergent in field theory [7]. In more detail, one considers the vacuum state and defines the subsystem A as a slab of length l in one of the spatial dimensions, at a fixed time slice. Then, the entanglement entropy contains, as its most divergent term, a term that is proportional to $|\partial A|/a^{d-1}$, where d is the number of spatial dimensions, a is the lattice spacing, and $|\partial A|$ is the area of the boundary surface between the slab and the rest of the space. To eliminate this divergence, which depends on details of the UV cut-off, one focuses on the entropic c-function [8]:

$$C(l) = \frac{l^3}{|\partial A|}\frac{\partial S_A}{\partial l}, \tag{2}$$

where we choose $d = 3$. $C(l)$ is a finite quantity even in the $a \to 0$ limit, and it becomes constant as a function of l in the conformal case.

In the present work, we non-perturbatively obtain the entropic c-function of SU(3) gauge theory, which describes the dynamics of gluons and has a confinement property. Although no analytic proof exists yet, accumulated numerical evidence implies that quantum chromodynamics (QCD) has a finite mass gap. At zero temperature, we expect from the asymptotic freedom that the entropic c-function is approximated by the contribution of non-interacting gluons at short distances l. On the other hand, at the hadronic scale, $l \sim \Lambda_{\mathrm{QCD}}^{-1}$, the entropic c-function captures the physics of confinement, or strong interactions. No analytical calculation of $C(l)$ seems possible in this region. In the limit $l \gg \Lambda_{\mathrm{QCD}}^{-1}$, the effective degrees of freedom responsible for the entanglement apparently reduce to non-interacting glueballs. It has been suggested [9] that the entropic c-function estimated by the correlation function of glueballs shows a Hagedron-type divergence. Furthermore, several works based on holographic and geometrical approaches found that S_A undergoes a quantum phase transition at $l_{\mathrm{cr}} \sim \Lambda_{\mathrm{QCD}}^{-1}$ [8–16]. At this critical value of l, the entropic c-function in the large N_c limit changes its behavior from $S_A \sim N_c^2$ at short distances to $S_A \sim N_c^0$ at long distances. Here, N_c is the number of colors.

There is a subtlety concerning the local gauge invariance of the entanglement entropy and of the Hilbert space for the subspace A on the lattice. Although several predictions and definitions for the entanglement entropy for the lattice gauge theory have been proposed [11,17–30], it turns out that some definitions give different values for the entanglement entropy. Recently, a definition that emphasizes the maximal gauge invariance has been proposed in Refs. [27,29]. The entanglement entropy in the replica method [19–22] agrees with that of the maximal gauge-invariant definition. In our work, we utilize the replica method following Refs. [19–22], and we obtain the entropic c-function numerically.

The replica method is a powerful technique for calculating the entanglement entropy. Based on this method, the entanglement entropy is given by the following equation:

$$S_A = \lim_{n \to 1}\left[-\frac{\partial}{\partial n}\ln\left(\mathrm{Tr}\rho_A^n\right)\right]. \tag{3}$$

Here, n is an integer, and it is referred to as a replica number. The period in the temporal direction for field variables in subsystem A is n times as long as that of subsystem B. The trace of the nth power of the reduced density matrix ρ_A is given by the ratio of the partition functions:

$$\mathrm{Tr}\rho_A^n = Z(l, n)/Z^n. \tag{4}$$

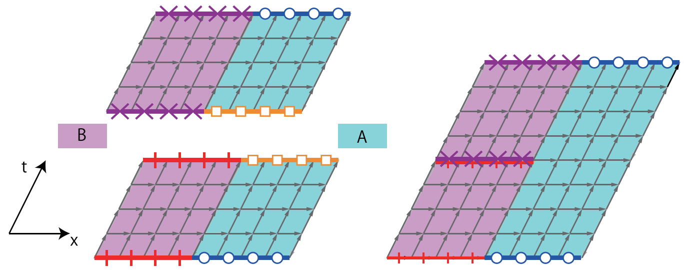

Fig. 1. Replica lattice and boundary conditions.

Here, Z is the original partition function for the whole system, and $Z(l, n)$ is the partition function for the system with an n-sheeted Riemann surface. The subsystem B is a patch of the nth Riemann surface while the subsystem A, whose length in one direction is l, is defined on a single Riemann surface.

Notice that Eq. (4) is directly related to one of the extended concepts of entanglement entropy, namely Rényi entropy $\left(S_A^n\right)$ [31,32]:

$$S_A^n = \frac{1}{1-n} \ln \mathrm{Tr}_{\mathcal{H}_A} \rho_A^n. \tag{5}$$

In the $n \to 1$ limit, it is back to the definition of entanglement entropy in Eq. (1).

The whole system is realized on a four-dimensional lattice of size $N_s^3 \times N_t$, with lattice spacing a, where N_s and N_t are the spatial and temporal lattice sizes, respectively. The system is divided into two subsystems, A and B, in the x-direction, and the numbers of sites in the x-direction of A and B are L and $N_s - L$, respectively. We adopt periodic boundary conditions for all directions. As explained above, the period of the temporal direction depends on the x coordinate. We show an example of the boundary condition on the replica lattice with $N_t = 4$, $n = 2$ in Fig. 1. In the figure, the boundaries with the same symbols in the t-direction are matched with each other via the periodic boundary condition. Thus, in subsystem B, the period of the temporal direction for the link variables is N_t (=4) in Fig. 1, while in A, it becomes $(n \cdot N_t)$. The boundary surface between A and B is extended in the y–z plane, and the area is given by $|\partial A| = (N_s a)^2$ in physical units.

The entropic c-function is obtained as the derivative of $\mathrm{Tr}\rho_A^n$ with respect to l and n. These derivatives are approximated by finite differentials with $(\Delta L) = 1$ and $(\Delta n) = 1$. We introduce the interpolating action [33,34] given by

$$\mathcal{S}_{\mathrm{int}} = (1-\alpha)\mathcal{S}_L[U] + \alpha \mathcal{S}_{L+\Delta L}[U], \tag{6}$$

where $\mathcal{S}_L$ and $\mathcal{S}_{L+\Delta L}$ represent the averaged action density on the replica lattices in which L and $L + \Delta L$ are the lengths of subsystem A. Here, U denotes the link variables, which are related to SU(3) gauge fields as $U_\mu(\vec{x}, t) = \exp\left[ig_0 A_\mu(\vec{x}, t)\right]$ with a bare coupling constant g_0. Now, we can rewrite Eq. (2) as

$$C(l) = \frac{L^3}{N_s^2 \Delta L} \int_0^1 d\alpha \left\langle \mathcal{S}_{L+\Delta L}[U] - \mathcal{S}_L[U] \right\rangle_\alpha, \tag{7}$$

where $\langle \cdot \rangle_\alpha$ refers to the Monte Carlo average with the interpolating action $\mathcal{S}_{\mathrm{int}}$ at a fixed value of α. We regard l in $C(l)$ as $(L + \Delta L/2)a$.

Table 1. Simulation parameters and the number of configurations for a $(N_s, N_t, n) = (16, 16, 2)$ lattice.

β	a [fm]	$L = 2$	$L = 3$	$L = 4$	$L = 5$	$L = 6$
5.700	0.1707	12 000	16 000	72 000	30 000	
5.720	0.1628			60 000		
5.740	0.1555			60 000		
5.750	0.1520	12 000	16 000	67 000	67 000	
5.770	0.1454			30 000		
5.780	0.1423			30 000		
5.800	0.1363	12 000	16 000	30 000	84 000	52 000
5.870	0.1182	12 000				

The strategy for calculating the entropic c-function using the lattice Monte Carlo simulation consists of five steps:

Step 1: Generate gauge configurations on the replica lattice using Monte Carlo simulation. The interpolating action $\mathcal{S}_{\text{int}}$ is used as a weight for the probability.
Step 2: Measure $\mathcal{S}_{L+\Delta L} - \mathcal{S}_L$ on each generated gauge configuration, and take an ensemble average of this for each value of α.
Step 3: Numerically integrate $\langle \mathcal{S}_{L+\Delta L} - \mathcal{S}_L \rangle_\alpha$ as a function of α.
Step 4: Take the continuum limit.
Step 5: Estimate the replica number dependence.

We utilize the standard Wilson plaquette action as an action, which has one coupling constant, namely the lattice bare coupling constant $\beta = 6/g_0^2$. Gauge configurations are generated by using the pseudo-heatbath algorithm. Thus, the link variables (U) are updated using the local interpolating gauge action $\mathcal{S}_{\text{int}}$ at a fixed value of α.

The details of simulation are as follows. The simulations were performed with a replica lattice volume $N_s^3 \times N_t = 16^4$ and $n = 2$. The simulation parameters and the number of generated configurations are summarized in Table 1. Each configuration is separated by 100 sweeps to avoid autocorrelation. We also show the value of the lattice bare coupling constant (β) and the corresponding length of the lattice spacing (a) in physical units. The pure Yang–Mills gauge theory is an asymptotically free theory, and it has only one physical scale, Λ_{QCD}. Once we fix a relation between a physical reference scale and a quantity in lattice units, then all physical quantities can be obtained in physical units. We use the relation between the lattice bare coupling constant and the lattice spacing given in Eq. (2.18) of Ref. [35]. Here, as a reference scale, we utilize the Sommer scale, in which the dimensionless static quark–antiquark force satisfies $r^2 F(r)|_{r=r_0} = 1.65$. To convert a quantity in lattice units into physical units, we assume that $r_0 = 0.5$ fm.

The error is estimated using the bootstrap method. First, we calculate $\partial S_A/\partial l$ for each bootstrap sample, and then estimate the statistical error from its distribution. The typical number of bootstrap samples constructed is $O(10^3\text{–}10^5)$.

In Steps 2 and 3, for each L, we take 11 points of α between $\alpha = 0.0$ and $\alpha = 1.0$, at intervals of $\Delta\alpha = 0.1$. The numerical integration is carried out using the cubic polynomial function. We also numerically investigated the dependence of $C(l)$ on the number of α points and the integration formula, and found that such effects are sufficiently smaller than the statistical uncertainty.

Figure 2 shows the result for the entropic c-function of the pure Yang–Mills theory at zero temperature. We found that the c-function is almost constant in the small l region ($l \lesssim 0.7$ fm); we fitted

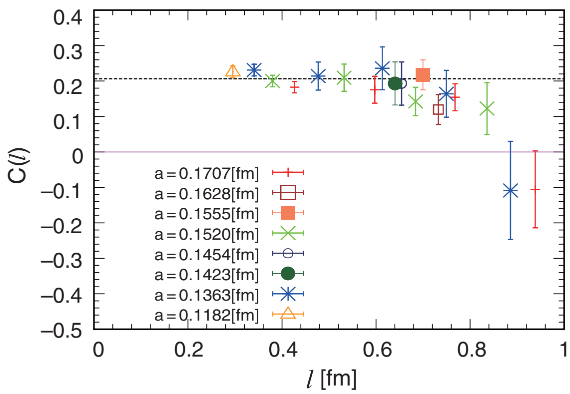

Fig. 2. Entropic c-function obtained by $(N_s, N_t, n) = (16, 16, 2)$ replica lattices. The dotted (black) line shows the best-fit value of $C = 2.06$.

the data with a constant for the data in the region $0 \leq l \leq 0.7$, and obtained the best-fit value

$$C = 0.206 \pm 0.007, \tag{8}$$

where the chi-square of the degrees of freedom is 0.88. Here, the error bars denote 1σ statistical error. To estimate the systematic uncertainty, we changed the range of the fit to $0 \leq l \leq 0.6$ and $0 \leq l \leq 0.8$, and obtained $C = 0.208(8)$ and $C = 0.202(7)$, respectively. The systematic uncertainty of C coming from the choice of the fit range is smaller than the statistical error.

The data shows continuous decrease in the middle l regime, and becomes consistent with zero beyond $l = 0.88$ fm. The critical temperature of the pure SU(3) Yang–Mills theory determined by the center symmetry breaking is $T_c = 280$ MeV, that is, $1/T_c = 0.714$ fm [36]. The Λ scale obtained from the running coupling constant based on the lattice simulation is $r_0\Lambda_{\overline{\text{MS}}} = 0.602(48)$ [35] and $r_0\Lambda_{\overline{\text{MS}}} = 0.613(2)(25)$ [37]. These correspond to $\Lambda^{-1}_{\overline{\text{MS}}} \sim 0.831$ fm and $\Lambda^{-1}_{\overline{\text{MS}}} \sim 0.816$ fm, respectively, when we set the Sommer scale $r_0 = 0.5$ fm. The length of l for which the c-function starts decreasing is in approximate agreement with these scales.

Next, let us compare our results with those found by other studies. A numerical simulation for the pure SU(2) gauge theory was carried out in Ref. [20]. In SU(2) gauge theory, the entropic c-function shows a clear discontinuity around $l = 0.5$ fm, and it shows an enhancement when the length is slightly less than this. These features are qualitatively different from those seen in SU(3).

Several holographic models also show a clear phase transition as a function of the distance l [8,9,13,14]. However, they are relevant to large-N_c Yang–Mills theories only. Furthermore, the value of l_c based on the free Hagedorn model is naively estimated to be $l \sim T_c^{-1}/2$ [9], in contrast to our result of $l \sim T_c^{-1}$. Interaction between glueballs might give correction terms.

Assuming that the monotonic decrease of the entropic c-function results from confinement, it is worth comparing the continuous behavior of the entropic c-function with another observation of confinement, namely, the static quark–antiquark potential. The lattice data for the static potential (see, e.g., the review paper [38]) reproduces the Coulomb potential of a quark–antiquark pair for short distances, which is seen in the perturbative picture. On the other hand, it shows a linear potential for long distances that is a signal of confinement. For intermediate distances, the lattice data smoothly connects the two regimes. Although we need further simulations to give solid evidence of the smooth change of the entropic c-function, our present results do not show a clear discontinuity and are analogous to the behavior of the static potential in the whole regime.

At short distances, the observed value of the entropic c-function, Eq. (8), can be understood reasonably well in terms of the degrees of freedom of gluons. First, we note in the case of SU(2) gauge theory that most of the data for $C(l)_{\mathrm{SU(2)}}$ at $l \leq 0.3$ fm (Fig. 6 in Ref. [20]) are located in the range $C = 0.07$–0.08.[1] Scaling down our value for Eq. (8) proportional to $\left(N_c^2 - 1\right)$, we obtain $C_{\mathrm{SU(2)}} \approx 0.077$.

Calculating the value of the entropic c-function for free gluon theory requires an independent quantitative discussion. The entanglement entropy in four-dimensional free theory is expressed as

$$S_A(l) = K|\partial A|\left[\frac{1}{a^2} - \frac{1}{l^2}\right]. \tag{9}$$

The coefficient $K \sim 0.0049$ [11] is obtained for the free real scalar theory. Assuming that the contribution of a free gauge boson is approximated with two real scalars, and taking into account eight color degrees of freedom in the SU(3) gauge theory, we get the following estimate:

$$C(l)_{\mathrm{free}} \sim 0.1568. \tag{10}$$

Keeping in mind the approximations made, the prediction in Eq. (10) falls remarkably close to our observed value, Eq. (8). The slight discrepancy may be caused by additional degrees of freedom, such as those due to glueballs, other excited states, or topological ground states in the lattice data, while Eq. (10) is obtained in a perturbative vacuum.

In the large-l regime, the data is consistent with zero. On the other hand, the free glueball analyses (e.g., Ref. [9]) show the exponential damping of the c-function as a function of the glueball mass beyond the Λ_{QCD} scale. Our data still have a large error and such behavior is not clear. We would like to examine the negative evidence of the discontinuity and the precise behavior beyond the Λ_{QCD} scale as future work.

We examine the validity of each analysis; in particular, we consider the finite volume effect, continuum extrapolation, and replica number dependence. To estimate the finite volume effect, we carried out a simulation with twice as large a lattice extent in each direction with fixed $(\beta, L, \Delta L)$. We found that the finite volume effects are negligible compared to the statistical error. Next, to estimate the discretization effects, we investigated the a dependence of the entropic c-function. Clearly, there is no a dependence, as shown in Fig. 2. Moreover, we carried out a simulation with a fixed physical lattice extent with half the lattice spacing. Although the statistical error is still large, the results with the halved spacing are consistent with the results shown in Fig. 2. The replica number dependence was studied by generating the data on an $n = 3$ replica lattice. The next-to-leading correction for the nth derivative of the entanglement entropy is smaller than the statistical error of our main results.

In summary, we present the first non-perturbative determination of the entropic c-function, which is the l-dependence of entanglement entropy in the SU(3) pure gauge theory, by using lattice QCD simulations. We utilize the replica method to obtain the entropic c-function, which is consistent with the maximally gauge-invariant definition. At short distances, the entropic c-function is proportional to the degree of freedom of gluons, and it is consistent with zero at long distances. In addition, the change between those two regimes occurs smoothly around a distance that is consistent with the QCD scale. Several systematic uncertainties are under control in our results.

For future work, we note that it will be straightforward to extend the present study to QCD with dynamical fermions. Although the exact order parameter for quark confinement is as yet unknown,

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the entropic c-function is expected to provide new insight into confinement from the viewpoint of the effective degrees of freedom. The application of this to finite temperature QCD will also be interesting. The entropic c-function at finite temperature gives the thermal entropy density in the long-distance limit. Preliminary results have already been presented in Ref. [22] and, as expected, these are roughly consistent with the results obtained by the other approaches [39]–[45]. Furthermore, determining the length of l at which the entanglement entropy density becomes consistent with the thermal entropy density would give a quantum correlation length for the quark–gluon plasma phase.

As another direction, several recent studies have found various conformal field theories for non-Abelian gauge theories by using a lattice numerical simulation to observe the non-perturbative running coupling constant [46–48]. Applying the present method to such conformal systems, the entropic c-function tells us the universal quantity related to the central charge for four-dimensional conformal field theories.

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