Deconfinement phase transition in the $SU(3)$ instanton-dyon ensemble

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Confinement remains one of the most interesting and challenging nonperturbative phenomena in non-Abelian gauge theories. Recent semiclassical [for $SU(2)$] and lattice (for QCD) studies have suggested that confinement arises from interactions of statistical ensembles of instanton dyons with the Polyakov loop. We extend studies of a semiclassical ensemble of dyons to the $SU(3)$ Yang-Mills theory. We find that such interactions do generate the expected first-order deconfinement phase transition. The properties of the ensemble, including correlations and topological susceptibility, are studied over a range of temperatures above and below T_c . Additionally, the dyon ensemble is studied in the Yang-Mills theory containing an extra trace-deformation term. It is shown that such a term can cause the theory to remain confined and even retain the same topological observables at high temperatures.

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I. INTRODUCTION

Quantum chromodynamics (QCD) is the quantum field theory describing the fundamental particles and forces that make up nuclear physics. While QCD is remarkably successful in describing nuclear physics, many phenomena remain beyond the scope of what can be studied analytically. Notably, nonperturbative phenomena such as confinement—the disappearance of quarks and gluons from the physical spectrum—is not completely understood. Confinement occurs not just in QCD but also in various Yang-Mills theories with or without quarks, making it clear that it emerges from the nonperturbative behavior of the gluons, rather than the quarks. Above a certain critical temperature T_c deconfinement takes place, and the QCD-like theories turn into a new form of matter, the quark-gluon plasma (QGP).

Historically the first mechanism of the deconfinement transition was a “dual superconductor” model [1–3]. At $T < T_c$ the chromoelectrically charged quarks and gluons are connected by QCD flux tubes, dual to magnetic flux tubes in superconductor. With the advent of lattice gauge theories many aspects of this scenario were put to the test. In particular, the profile of the QCD flux tubes [4] was found to agree well with the dual superconductor model. Monopoles were observed and found to rotate around these flux tubes, as expected. Bose-Einstein condensation of

monopoles was detected and its critical temperature was shown to coincide with T_c [5]. A high density of monopoles was found to be responsible for unusual kinetic properties of QGP [6].

Euclidean formulation of the gauge theory led to the discovery of 4D topological solitons known as Belavin-Polyakov-Schwarz-Tyupkin instantons [7]. A model of their ensemble, the instanton liquid model [8], has explained how instantons generate chiral symmetry breaking. As certain extrema of the path integral over gauge configurations, they form a basis for semiclassical theory, consistently including fluctuations around classical fields. Furthermore, one can study the interaction between instantons in their statistical ensemble: those studies explained behavior of correlation functions of various mesonic and baryonic currents; for a review see, e.g., Ref. [9]. Yet the instanton theory has not reproduced confinement.

Euclidean formulation of finite temperature QCD naturally led to a nonzero value of the Polyakov loop ($\langle P \rangle \neq 0$) as a signature of deconfinement. Note that throughout this paper we use $\langle P \rangle$ as shorthand for $\frac{1}{3} \langle \text{Tr}[\hat{P}(\vec{x})] \rangle$. It can be interpreted as the nonzero vacuum expectation value (VEV) of the Euclidean time component of the gauge field A_4 , also known as *nonzero holonomy*. The natural question was then how to deform the instanton configurations in a manner consistent with nonzero holonomy in the bulk. It was answered in Refs. [10,11], who discovered that instantons dissolve into N_c (number of colors) constituent solitons, called *instanton dyons* (or instanton monopoles). Like original instantons, they are (anti-)self-dual, so their actions and topological charges are equal. But, unlike instantons, their actions and topological charges are *not* quantized to integers; standard index theorems are avoided because

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instanton dyons have magnetic charges and therefore are still connected by Dirac strings.

It was then realized that instanton dyons provide a very valuable bridge between the theory of monopoles and instantons, providing a way to explain *both* confinement and chiral symmetry breaking in a single setting. Unlike monopoles, instanton dyons are semiclassical objects, allowing for the construction of a consistent theory of an interacting ensemble. Last but not least, the statistical sum in terms of instanton dyons is “Poisson dual” to that based on monopoles; see Refs. [12,13].

Semiclassical approaches to finite- T gauge theories, with and without quarks, have lately been the subject of multiple studies. Confinement in this theory is due to the backreaction of the dyon ensemble on the Polyakov loop, forcing it to take a zero value at $T < T_c$; see, e.g., Ref. [14] for a simple model, Ref. [15] for mean-field analysis, and Refs. [16,17] for numerical simulations of the $SU(2)$ gauge theory. It is important that they are semiclassical objects, unlike the QCD monopoles [13], with the actions $S_{\text{dyons}} \sim 1/g^2 \sim \log(T/\Lambda)$ growing with temperature. Therefore, their densities are suppressed at high T as an inverse power of T . At temperatures comparable to the critical one, $T \sim T_c$, numerically $S_{\text{dyons}}/\hbar \approx 4$. The inverse of it is the small parameter of our semiclassical expansion.

Although in this work we study pure gauge theory rather than QCD-like theories with light quarks, let us mention that the instanton-dyon ensemble also describes the breaking of chiral symmetry. Numerical studies of chiral phase transition can be found in Refs. [18,19]. Using light quark Dirac eigenstates, one can identify the individual dyons inside lattice configurations from large-scale QCD simulations. As shown recently [20], the lowest Dirac states are indeed generated by the instanton dyons, in a form that is remarkably insensitive to large density of perturbative quarks and gluons in which they are immersed.

In this work we extend the studies [16,17] to the pure $SU(3)$ gauge theory. Instead of two species of instanton dyons, we now deal with three. It is well known from lattice studies [21] that the pure $SU(3)$ gauge theory [and all pure $SU(N_c)$ theories with $N_c \geq 3$] possesses a first-order phase transition rather than the second-order transition seen in $SU(2)$. So the question that we address below is whether this and other features of pure $SU(3)$ gauge theory can be reproduced by the instanton-dyon ensembles.

This paper is structured as follows: The dyon interactions and partition function are discussed in Sec. II. Section III lays out some technical details of the simulation as well as the data analysis performed. The physical results, including correlation functions and the temperature dependence of parameters such as the Polyakov loop, are shown in Sec. IV. Finally, in Sec. V, the deconfinement transition of the dyon ensemble is studied in the trace-deformed Yang-Mills theory.

II. INSTANTON DYONS IN THE $SU(3)$ GAUGE THEORY

A. Dyons and holonomy

The Polyakov loop is an order parameter of the deconfinement phase transition,

$$\hat{P} = \text{P exp} \left(i \oint A_4^a T_a d\tau \right), \quad (1)$$

where T^a is the color generator in the fundamental representation and P indicates the path-ordered product. Then $\hat{P}$ is a unitary matrix with phases for eigenvalues, so A_4 can be defined as $A_4 = 2\pi T \text{diag}(\mu_1, \mu_2, \mu_3)$. These phases are related to the holonomies of the dyons by $\nu_i = \mu_{i+1} - \mu_i$, where $\mu_{i+1} > \mu_i$ and $\mu_4 = \mu_1 + 1$. The connection between the Polyakov loop and confinement can be seen through its relation to the free energy of a static quark,

$$\langle P \rangle = e^{-F_q/T}. \quad (2)$$

Clearly, $\langle P \rangle = 0$ is the confining holonomy corresponding to $F_q \rightarrow \infty$.

For $SU(N_c)$ gauge theories, there are N_c types of dyons: $N_c - 1$ of them are called M_i -type dyons, they correspond to the maximal diagonal subgroup. Another type is called the “twisted” (that is, time-dependent) or L -type dyon. There are corresponding antidyons as well, giving in total $2N_c$ species of dyons. Note that we will use *species* to refer to one of the six dyons and *type* to refer to one of the three pairs of a dyon and its antidyon (i.e., an M_1 -type dyon refers to both M_1 and $\bar{M}_1$ dyon species). The action of each individual dyon of type i is denoted by $S_0 \nu_i$, where ν_i are the so-called holonomy parameters. They are also called “fractions of the holonomy circle” because they satisfy the sum rule,

$$\sum_i^{N_c} \nu_i = 1,$$

and *generically* have $N_c - 1$ independent parameters. These holonomy parameters determine not only the actions but also the core sizes of the dyons: $r_i \sim 1/(2\pi\nu_i T)$. In $SU(N_c)$ theories, (anti)instantons comprise one of each type of (anti)dyon, although this is not necessarily the case for other gauge groups. For example, in $SU(3)$, the instanton $I = M_1 L M_2$ and the anti-instanton $\bar{I} = \bar{M}_1 \bar{L} \bar{M}_2$.

The main parameter defining the properties of the dyons is the classical instanton action

$$S_0 = \frac{8\pi^2}{g^2} \sim \log(T)$$

containing the coupling at the temperature-dependent scale. While this parameter is independent of the holonomy, the

FIG. 1. Structure of the holonomies and dyon types in $SU(3)$. The circle has a circumference of 1.

actions of individual dyons of type i are $S_i = S_0 \nu_i$. In the $SU(2)$ case, one defines one holonomy parameter $\nu \in [0, 1]$, the M dyon having action $S_M = S_0 \nu$, and the L dyon having the conjugate action $S_L = S_0(1 - \nu)$. In the $SU(3)$ case there are two diagonal Gell-Mann matrices, λ^3 and λ^8 , and in principle two holonomy parameters. However, the average Polyakov loop $\langle P \rangle$ is a gauge-invariant, and thus physical, object. Restricting it to be *real* enforces $\nu_{M1} = \nu_{M2}$, thereby reducing the holonomy to just a single parameter for $SU(3)$ with $\nu \in [0, 1/2]$.

When the previous definitions of the holonomies and phases are combined, the relationship between the holonomy and the average Polyakov line is found to be

$$\langle P \rangle = \frac{1}{3} + \frac{2}{3} \cos(2\pi\nu). \quad (3)$$

From this it is clear that $\nu = 1/3$ is confining ($\langle P \rangle = 0$), while $\nu \rightarrow 0$ produces the “trivial” Polyakov loop ($\langle P \rangle = 1$).

The dyon actions expressed in terms of it are

$$S_{M1} = S_{M2} = S_0 \nu, \quad S_L = S_0(1 - 2\nu), \quad (4)$$

and the relation between this holonomy parameter and the phases μ_i can be seen in Fig. 1. This symmetry between the M_1 - and M_2 -type dyons means that they have equal densities as well, thus greatly reducing the space of parameters that needs to be considered.

B. The partition function and dyon interactions

To start, let us note that all interactions of the dyons contain the dimensionless distance rT rather than the dimensionful distance r . For this reason we define many quantities in terms of this dimensionless distance: the dimensionless 3-volume $\tilde{V}_3 = V_3 T^3$, the dyon densities $n_i = \frac{N_i}{\tilde{V}_3}$, and the free energy density $f = \frac{F}{\tilde{V}_3 T}$ where $F = -T \ln(Z)$ is the (dimensionful) free energy and N_i , $i = M_1, M_2, L$ are the numbers of each species of dyon.

A complete calculation of the dyons’ free energy requires the construction of the dyonic partition function. We start with effects that are not induced by the dyons’ nonperturbative interactions. In the absence of all dyonic effects, there is a perturbative interaction between thermal gluons and the holonomy. This generates the Gross-Pisarski-Yaffe potential V_{GPY} [22], which appears in the exponent of the partition function. For $SU(3)$, this is given by

$$\frac{V_{\text{GPY}}}{T \tilde{V}_3} = \frac{4\pi^2}{3} (2(\nu(1 - \nu))^2 + (2\nu(1 - 2\nu))^2). \quad (5)$$

Here the potential is shown with factors divided out so that it has units of free energy density. This potential disfavors confinement, having a minimum at the trivial holonomy $\nu = 0$ and a maximum at the confining holonomy $\nu = \frac{1}{3}$.

The dyon contribution to the partition function consists of two parts, the contributions of the dyons in the absence of interactions Z_0 , which can be expressed analytically directly from the input parameters, and Z_{np} , the contributions of the dyon interaction, whose calculation is the subject of the simulation of the partition function (performed using Monte Carlo algorithms in this work). The total partition function is their product $Z = Z_0 Z_{np}$.

The statistical weight for a single instanton was explicitly calculated in Ref. [23] for $SU(2)$. Taking the dilute limit, which removes the interaction between the dyons, this gives

$$Z_0^{SU(2)} = \frac{\Lambda}{(4\pi)^2} S_0^4 e^{-S_0^2 \nu^{\frac{8}{3}-1}} (1 - \nu)^{\frac{8(1-\nu)}{3}-1}. \quad (6)$$

It is easy to see how this factors into the weight for each individual dyon: Each dyon species contributes a factor of $\sqrt{\Lambda} S_0 e^{-\sqrt{S_0} \nu}$ and the two holonomy terms stem from the holonomies of the individual M - and L -type dyons. A factor of $4\pi \nu_i$ is divided out for each dyon type. This is to remove a constant term that remains when taking the dilute limit in Z_{np} . Knowing this, it is easy to construct the instanton weight in $SU(3)$ and extend it to an arbitrary number of dyons by summation. The partition function, assuming an equal number of dyons and antidyons, is

$$Z_0 = \sum_{N_{M1}, N_L, N_{M2}} \left(\frac{1}{N_{M1}!} (\tilde{V}_3 d_\nu)^{N_{M1}} \right)^2 \times \left(\frac{1}{N_L!} (\tilde{V}_3 d_{1-2\nu})^{N_L} \right)^2 \times \left(\frac{1}{N_{M2}!} (\tilde{V}_3 d_\nu)^{N_{M2}} \right)^2, \quad (7)$$

where d_ν is the weight of an individual dyon with holonomy ν ,

$$d_\nu = \frac{\Lambda}{4\pi} S_0^2 e^{-S_0 \nu} \nu^{\frac{8\nu}{3}-1}. \quad (8)$$

Now we may take the limit $V \rightarrow \infty$ and assume equal densities of M_1 - and M_2 -type dyons. Additionally we resolve the factorial terms with Stirling's approximation carried out to three terms $\ln N! \approx N \ln N - N + \ln(\sqrt{2\pi N})$. The free energy $F = -\ln(Z)$ is given by the following expression:

$$f = \frac{4\pi^2}{3} (2(\nu(1-\nu))^2 + (2\nu(1-2\nu))^2) - 4n_M \ln \left[\frac{d_\nu e}{n_M} \right] - 2n_L \ln \left[\frac{d_{1-2\nu} e}{n_L} \right] + \frac{\ln(8\pi^3 N_M^2 N_L)}{\tilde{V}_3} + \Delta f, \quad (9)$$

where Δf is the free energy density stemming from the interactions of the dyons. If the dyons have classical binary interactions ΔS_{class} and a volume metric G , their contributions to the partition function and the free energy density are

$$Z_{np} = \frac{1}{\tilde{V}_3^{(4N_{M1}+2N_L)}} \int Dx \det(G) e^{-\Delta S_{\text{class}}} \quad (10)$$

$$\Delta f = -\ln(Z_{np}) \quad (11)$$

The set of parameters that minimizes the free energy density corresponds to the physical dyon ensemble in the infinite-volume limit. This elucidates the main procedure of this work: to first compute the free energy density of the ensemble for a wide range of parameters, and then to locate their values which minimize it.

The classical interactions between dyons and antidyons are, at distances exceeding the dyon cores, asymptotically Coulomb-like. For generic $SU(N_c)$ theories, the interactions are given in Ref. [24]. At shorter length scales, the interaction is modified. The interaction between dyons and antidyons of the same type was studied in detail and parametrized by Larsen and Shuryak [25]. In this work, a gradient flow method was used to minimize the action of an M - $\bar{M}$ pair on the lattice giving a set of “streamlined” configurations. The minimized action as a function of the dyon separation reveals the classical interaction potential between the dyons (see Fig. 6 in Ref. [25]), which was parametrized. A different parametrization following from the same data was used in the numerical studies of the $SU(2)$ ensemble [16]. We use a parametrization similar in form to the latter for all dyon-antidyon pairs,

$$\Delta S_{\text{class}}^{d\bar{d}} = -\frac{S_0 C_{d\bar{d}}}{2\pi} \left(\frac{1}{rT} - 2.75\pi \sqrt{\nu_i \nu_j} e^{-1.408\pi \sqrt{\nu_i \nu_j} rT} \right), \quad (12)$$

where $C_{d\bar{d}}$ is a coefficient with value 2 for pairs of the same type and -1 for pairs of different types. Compared with the parametrization used in $SU(2)$, the coefficient in front of the exponential term has been reduced from its original value of 3.264 and the substitution $\nu_i \rightarrow \sqrt{\nu_i \nu_j}$ was made to accommodate pairs of dyons with different holonomies (e.g., $M_1 L$) to improve the behavior of some observables. These interactions are used for distances greater than the core size $r_0 = x_0/(2\pi\nu T)$. Dyon pairs of the same type (regardless of duality) experience a repulsive core. While the core potential has not been studied in detail, it is reasonably described by

$$\Delta S_{\text{class}}^{\text{core}} = \frac{\nu V_0}{1 + e^{2\pi\nu T(r-r_0)}}. \quad (13)$$

The two parameters in this interaction, x_0 and V_0 , are chosen on a phenomenological basis and should be subject to constraints from appropriate lattice data when possible. See Appendix B for a discussion of their values and the effects of changing them.

Additionally, the dyons experience an effective potential from the fluctuation determinant of the instanton. This effect leads to the following Diakonov determinant [26] of the metric of the space of the dyons' collective variables:

$$G_{im,jn} = \delta_{ij} \delta_{mn} \left(4\pi\nu_m - \sum_{k \neq i} \frac{2}{T|r_{i,m} - r_{k,m}|} + \sum_k \frac{1}{T|r_{i,m} - r_{k,p \neq m}|} \right) + \frac{2\delta_{mn}}{T|r_{i,m} - r_{j,n}|} - \frac{1 - \delta_{mn}}{T|r_{i,m} - r_{j,n}|}, \quad (14)$$

where $r_{i,m}$ is the position of the i th dyon of type m . This metric accounts only for the self-dual dyons. An equivalent metric $\bar{G}$ is used for the antidyons. The metric is true for dyons of different species at any distance, but true only at larger distances for dyons of the same species. We modify the terms with a cutoff $r \rightarrow \sqrt{r^2 + (3/2\pi T)^2}$ so that the diagonal entries go to 0 rather than $-\infty$ when $\nu = \frac{1}{3}$. The effective potential from this metric comes as

$$\Delta S_{1\text{-loop}} = -\ln(\det G \det \bar{G}). \quad (15)$$

The diagonal of this metric does not vanish in the dilute limit, instead going to $\prod_i 4\pi\nu_i$. This has been accounted for by modifying the individual dyon weight in Eq. (8).

It is observed that if the densities of different dyon types are unequal, then in the infinite-volume limit, the sum diverges. We therefore regulate all Coulomb terms in both the classical and one-loop potentials with the dimensionless Debye mass $r \rightarrow re^{M_D r T}$. Like the core parameters, the

value of the Debye mass is a choice that should be subject to improvement.

Now let us give a brief qualitative discussion of how such interactions should generate confinement. The main interaction driving confinement is the repulsive cores of the dyons. Because the volume of the cores goes as $1/\nu^3$, this interaction disfavors any type of dyon becoming large and thus favors the confined phase $\nu = \frac{1}{3}$, where all dyons are the same size. The long-distance classical Coulomb interactions disfavor confinement, however. Because dyons repel anti-dyons of different types but attract anti-dyons of the same type, these interactions favor ensembles with many dyons of the same kind (a large value of n_M/n_L) rather than equal numbers of all species. At larger values of n_M/n_L the entropy portion of the partition function Z_0 more strongly favors small values of ν , driving the system to the deconfined phase. The one-loop Coulomb-like interactions have the opposite sign and thus the opposite effect. These one-loop interactions are suppressed by a factor of S_0 and are comparable only to the classical interactions at low T . At low T , the cores are the dominant contribution to the free energy, while at high T the dyon density falls and V_{GPY} shifts the system to the deconfining holonomy.

III. THE SIMULATION SETTING AND DATA ANALYSIS

Numerical integration over the dyons' coordinates is performed using Monte Carlo techniques. The position of each dyon is updated and then accepted or rejected according to the standard Metropolis algorithm. Once this is done for each dyon five times (five updates is approximately the autocorrelation time of the ensemble), the configuration is sampled and its properties are computed. The free energy is obtained via the usual integration over auxiliary parameter λ ,

$$e^{-F(\lambda)/T} = \int D\mathbf{r} e^{-\lambda S}, \quad (16)$$

$$\Delta F = \int_0^1 d\lambda T \langle \Delta S \rangle, \quad (17)$$

where this nonperturbative free energy is added to the perturbative contribution from Eq. (9). Integration over the dummy parameter is performed in ten equal steps $\lambda = 0.1, \dots, 1$, with the average energy at each step computed from 2000 configurations. Because the contribution at small λ is large, the value of the average interaction at $\lambda = 0$ is obtained from a linear fit of the nearest points and included in the numerical integration. With all of this, the statistical uncertainty in the computations of f are generally at the percent level.

The goal of these simulations is to calculate the free energy density f of ensembles with three main input parameters, the holonomy ν , and the dyon densities n_M ,

n_L over a range of temperatures near T_c . All simulations are performed with a fixed number of dyons $N_D = 120$ or 122 (60 or 61 dyons and 60 or 61 anti-dyons). For the six species of dyons in $SU(3)$, $N_D = 4N_M + 2N_L$. The system is studied on a flat geometry with finite density imposed by a periodic box surrounded by 26 image boxes, as was done for $SU(2)$ in Ref. [17]. The densities of the dyons, n_M and n_L , are controlled by varying the size of the box and the ratio of the numbers of each type of dyon N_M/N_L for a specific value of N_D . Two values of N_D are used to allow for more values of N_M/N_L to be used.

There are two technical details of the simulation that must be mentioned. The first is the Diakonov determinant $\det G$, which is not positive definite for randomly placed dyons. It was shown by Bruckmann *et al.* [27] that, in fact, at reasonable densities, nearly all random configurations have at least one negative eigenvalue λ_i . This is handled by a modification of the effective potential

$$\Delta S_{1\text{-loop}} = \begin{cases} -\ln(\det G \det \bar{G}) & \text{if } \lambda_i \geq 0 \forall i, \\ V_{\text{max}} & \text{otherwise,} \end{cases} \quad (18)$$

where V_{max} is a large value (we choose $V_{\text{max}} = 100$) which serves to reject all Metropolis updates into the region of negative eigenvalues. The choice of V_{max} is arbitrary as long as it is large enough to ensure that no configuration with negative eigenvalues is accepted during the course of the simulation.

The second is an approximation which must be made due to computational resources. The total system, the main box and all its nearest images, contains $27N_D$ dyons. Its 2D version is shown in Fig. 2. The most demanding step in the simulation is the computation of $\det G$ which is an $\mathcal{O}(N^3)$ process. Performing this computation at every update step of the Metropolis algorithm is numerically costly given the large number of parameters for which the free energy must be calculated. Instead, the change in action associated with each update is computed considering only the dyons in a box of the same size as the simulation box centered at the position of the dyon being updated. This approximation is well justified by the fact that all long-range interactions are regulated by a Debye screening length.

Once the free energy density of each set of parameters is determined, a fit is performed to determine the dependence of the free energy density near the minimum. For each value of the action S_0 there is a three-dimensional space of input parameters with coordinates (ν, n_M, n_L) . The points near a minimum are fit to a quadratic function in these coordinates. From the fit, the minimum value of f and its location in the coordinate space is determined. For every value of S_0 tested, all local minima are identified and the points near them are fit as described. The fit with the lowest minimum value of f is the global minimum. For cases where a minimum is located in the confined phase with $\nu = \frac{1}{3}$ and $n_M = n_L$, these equalities are assumed to be

FIG. 2. Schematic depiction of the main simulation box (center) and surrounding images setup. The dashed box shows the volume containing all dyons whose interactions are considered in the Metropolis update step of the dyon represented by a square point. Such a volume always contains N_D dyons.

exact and the minimum is fit to a quadratic function only in n_M .

In summary, the results presented in this work are obtained using the following procedure: (i) Perform simulations over a wide range of parameters ν , n_M , n_L for each temperature tested. (ii) Determine the global minimum for each temperature via fitting to determine the physical values of these parameters: $\nu(T)$, $n_M(T)$, and $n_L(T)$. (iii) Study the ensembles with the physical values with increased statistics to compute correlations and topological charge distributions. (iv) With these increased-statistics runs, we generate 80,000 configurations with the physical interactions between them ($\lambda = 1$; we no longer need to integrate over it) using the fitted values of the inputs for each temperature studied.

IV. RESULTS

A. Structure of the holonomy potential and the phase transition

It is expected that the pure $SU(3)$ gauge theory will possess a first-order phase transition at some critical temperature T_c . The dyon interactions generate the holonomy potential, which has a global minimum in the confined phase at $T < T_c$ and then a jump to a new global minimum in the deconfined phase at $T > T_c$. The first goal of this work was to check for the existence of such a phase transition. Parameters of the interaction were chosen so that this would occur at around $S_0 \sim 12$ (see Appendix B for more details). For each value of the temperature, which is related to S_0 by Eq. (A1), the shape of the holonomy

potential was computed and the minimum was determined. The value of the holonomy and dyon densities at which this minimum occurs are the physical values that the ensemble takes on at that temperature.

The instanton action S_0 was varied in steps of 1 from $S_0 = 8 - 21$ and the other parameters were varied as shown in Table I. It was observed that the phase transition occurs when $13 < S_0 < 14$, and additional simulations were performed at $S_0 = 12.75, 13.25, 13.5$, and 13.75 to locate the critical temperature more accurately. A linear fit was performed to the free energy density with the nearest points on both sides of the transition to determine that the phase boundary is located at $S_0 = 13.18$. With this, the action can now be rewritten in terms of T/T_c . The range of temperatures studied here is then $0.62T_c < T < 2.04T_c$. In physical units, this is approximately $160 \text{ MeV} < T < 530 \text{ MeV}$.

This model of the dyon interactions relies on a semiclassical expansion. An important consideration is then to determine whether the main semiclassical quantity, the action of the dyons $S_i = S_0\nu_i$, remains sufficiently large over this temperature range. In the confined phase, all dyons have the action $S_0/3$, meaning that there is clearly a lower bound where the action becomes small and we choose $S_0 = 8$, $S_i = 2.6$ as a reasonable lower bound. In the deconfined phase, as the instanton action grows, the holonomy decreases, making the action of the M_i -type dyons the limiting factor. The action of these dyons remains nearly constant at $S_M \simeq 3$ up to $2T_c$. Thus, the dyons remain sufficiently semiclassical throughout the entire range of temperatures studied.

When linear fits to data points near the transition are performed, all parameters of the ensemble can be determined on both sides of the phase transition. Table II

TABLE I. Input parameters used for the main simulation runs. Some additions and changes were made as needed. (Some noninteger values of S_0 were added near T_c and the values of n_M were increased at lower temperatures.)

	Min.	Max.	Step size	No. of steps
S_0	8	21	1	14
ν	0.1	0.35	$0.01\bar{6}$	16
n_M	0.15	0.6	0.03	16
N_M/N_L	1.0	30.0	Varied	16

TABLE II. Values of the parameters of the ensemble above and below the critical temperature T_c from linear fits to the nearest data points on either side of the phase transition at $S_0 = 13.18$.

	$T \rightarrow T_c^-$	$T \rightarrow T_c^+$
ν	$1/3$	0.236
$\langle P \rangle$	0	0.392
n_M	0.550	0.529
n_L	0.550	0.068

FIG. 3. Holonomy dependence of the free energy density for different values of the M -dyon density n_M in both phases. Left panel: confined phase with $S_0 = 12.75$, $n_L = n_M$. Right panel: deconfined phase with $S_0 = 13.75$, $n_L = n_M/9.6$. Error bars are omitted for readability.

summarizes these values. From the table it is clear that the transition is first order—the holonomy/Polyakov loop and both dyon densities are discontinuous at the phase boundary. While the fits are done on just 2 or 3 points on either side of T_c , the uncertainties in these values should be about the same magnitude as the individual points—at the percent level.

At temperatures below T_c the ensemble is in the confined phase with $\nu = 1/3$ and $n_M = n_L$, as can be seen in Fig. 3 (left panel). At densities below the physical one, the minimum shifts to the left as the nonperturbative interactions become weak relative to the perturbative contribution to the free energy. At higher densities the ensemble prefers to remain in the confined phase, but with a larger free energy minimum and curvature of the potential.

The deconfined phase has a similar structure, but with the global minimum occurring at $\nu < 1/3$ and $n_M > n_L$. However, at densities above that of the global minimum, the minima continue to move toward larger ν . At these densities, the repulsive core dominates and it becomes energetically favorable to make the many M_i dyons smaller at the cost of making the few L dyons larger. It is possible that at densities higher than those studied here, the ensemble may have a minimum at $\nu > 1/3$.

These plots show a slice of the full space of parameters explored for each value of S_0 only for specific values of n_M/n_L . The structure of the first-order phase transition can be seen more clearly in Fig. 4. By considering the minimum free energy density selected from all combinations of n_M and n_L as a function of the holonomy, the two local minima—one in the confined phase and the other in the deconfined—are clearly visible. At the value of S_0

nearest the critical value, the free energy at the two minima are nearly degenerate and the global minimum switches between the two as the temperature crosses T_c .

This structure is different from the that of $SU(2)$. In $SU(2)$, where the phase transition is second order, rather than having two degenerate minima, the holonomy potential flattens near T_c (see, e.g., Fig. 5 of Ref. [16]). This allows the minimum to quickly but smoothly shift from the confining holonomy to smaller values. Additionally, there is a $\nu \leftrightarrow 1 - \nu$ symmetry that is not present in $SU(3)$.

FIG. 4. Holonomy dependence of the minimum free energy density near the phase transition. Error bars are omitted for readability.

FIG. 5. Temperature dependence of the free energy density of the dyon ensemble.

B. Temperature dependence of the parameters

The free energy density f , unlike other physical quantities, remains continuous across even a first-order phase transition, as we see in Fig. 5. Its derivative, however, may not. The free energy varies with temperature much more rapidly in the confined phase than the deconfined.

The most important feature of the dyon ensemble for describing the deconfinement transition is the average Polyakov loop as a function of the temperature $\langle P(T) \rangle$. Below T_c , the holonomy takes the confining value $\nu = 1/3$, $\langle P \rangle = 0$. At T_c the value jumps to ~ 0.4 and then continues to increase as T increases. The value of the average Polyakov loop above the phase transition shows qualitative agreement with the lattice data for the *renormalized* Polyakov loop [21], but it does not increase with temperature as quickly, as shown in Fig. 6. A change to the parameters of the dyon interactions could improve the agreement with the lattice data.

Another set of properties of the ensemble involves the densities of each dyon type (shown in Fig. 7). At $T < T_c$, all densities are equal, reflecting the fact that, in the confined phase, all dyons have equal statistical weights, core sizes, and masses and have symmetric interactions between them. At $T > T_c$, the holonomy decreases discontinuously, causing a similar change in both dyon densities. In the case of the M -dyon density n_M , the decrease in ν increases the statistical weight of the M_i -type dyons while simultaneously increasing the size of their repulsive cores. These competing effects result in what is seen in the ensemble: a small [$\mathcal{O}(5\%)$] decrease in n_M at the phase transition. The L -dyon density sees a more

FIG. 6. Temperature dependence of the average Polyakov loop of the dyon ensemble. The lattice data are taken from Ref. [21] and shown without error bars. Errors in the lattice data have magnitudes comparable to those in the dyon data.

significant decrease due to the large decrease in statistical weight of the L dyons from the increase in $1 - 2\nu$.

Overall, the dyon densities decrease with temperature, which is consistent with the expected behavior of instantons. It is the dyon densities that set the upper limit on the temperature that can be studied in our ensemble.

FIG. 7. Temperature dependence of the densities of each type of dyon in the ensemble.

As temperature increases, the ratio n_M/n_L becomes larger and larger, and, at the largest values, the number of L dyons in the simulations is just 1 or 2. The small number of L dyons makes fitting near the free energy minimum in n_L difficult, as their contribution to f is vanishingly small. Thus, our upper limit ($S_0 = 21$) is a technical constraint rather than a physical one; accurately probing higher S_0 would require a larger ensemble with better statistics.

C. Spatial correlations between dyons

It is useful to study the effects of the dyons' interactions by studying the spatial correlations between them. Such correlations will be useful for comparison to studies of the dyons in lattice configurations. The most straightforward characteristic of the spatial correlations are the correlation functions $C_{ij}(rT)$ between two dyons of species i and j . In $SU(3)$, because the instanton comprises three constituent dyons, it is useful to also define the “instanton correlation function” $C_I(yT)$, where y is the hyperdistance in the six-dimensional space of Jacobi coordinates of the three dyons,

$$y^2 = \frac{1}{3}(r_{M1,L}^2 + r_{M1,M2}^2 + r_{L,M2}^2). \quad (19)$$

In both cases, the functions are normalized such that C_{ij} , $C_I \rightarrow 1$ at large (hyper)distance and have had the angular factors divided out [$(rT)^2$ for the two-dyon correlation functions and $(yT)^5$ for the instanton correlation function].

Many of the correlation functions are redundant, so we need to observe only a subset of the correlation functions to understand the behavior of the ensemble. Figure 8 shows these functions in both phases. The strongest correlation between the dyons is seen in the instanton channel where

the three constituent dyons have positive short-range correlation due to the attractive terms in the Diakonov determinant.

In several channels we can clearly see the effects of the repulsive core at short ranges. In the $D\bar{D}$ channels, we can see positive correlation just beyond the cores. Changes in the cores can also be seen: in the $M_1\bar{M}_1$ channel, the core becomes larger and softer above T_c , soft enough that many pairs can still be found at $x < x_0$, while the cores of the L dyons becomes smaller and harder, thus reducing the correlation function to 0 at $x < x_0$. The smaller core size also allows the attractive long-range interactions to become larger near the core, enhancing the correlation found there.

Despite having no long-range interactions, there is small correlation seen in the same-species (M_1M_1 and LL) channels beyond the core due to some mutual correlations to other dyons. Compared to that in the $D\bar{D}$ channels, the anticorrelation at small r is even stronger due to additional repulsion from the Diakonov determinant. Some correlation functions for the dyons in pure $SU(3)$ Yang-Mills theory at $T/T_c = 0.96$ have been observed in lattice configurations [28]. We find qualitative agreement with these results in all channels except for dyons of the same species. Here some short-range correlation is observed among the lattice dyons, suggesting an absence of the repulsive core used in our model in this channel.

D. The vacuum angle and moments of the topological charge

Another set of important characteristics of the dyon ensemble involves its topological properties. Non-Abelian gauge configurations generically may possess some topological charge Q with its density $q(x)$ given by

FIG. 8. Spatial correlations of the dyons in the $M_1\bar{M}_1$ (upper right panel), $L\bar{L}$ (upper middle panel), $M_1\bar{L}$ (upper right panel), M_1M_1 (lower left panel), LL (lower middle panel), and instanton (lower right panel) channels above and below the phase transition.

FIG. 9. Distribution of values of the total topological charge Q in the half boxes at $S_0 = 12$ ($T/T_c = 0.898$).

$$q(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x). \quad (20)$$

The (anti)instantons are topologically nontrivial objects with $Q = \pm 1$. The constituent dyons then each carry some fraction of this charge. Dyons of species i carry topological charge $Q = \nu_i$, while antidyons have charge $Q = -\nu_i$. Because we consider only ensembles with equal numbers of dyons and antidyons, and thus equal positive and negative topological charges, the average topological charge $\langle Q \rangle$ is zero in any subvolume of the box, while higher moments are not. The most prominent topological feature of the gauge theory, which has been extensively studied on the lattice [29–31], is the (dimensionless) topological susceptibility $\chi = \langle Q^2 \rangle / \tilde{V}_4$, where $\tilde{V}_4 = (LT)^3(\beta T)$ is the four-dimensional space-time volume of the system. In our dimensionless notation the Euclidean time circle has circumference $\beta T = 1$, so $\tilde{V}_4 = \tilde{V}_3$.

Because the dyons in our semiclassical ensemble have well-defined positions and topological charges, measuring the average topological charge requires summing only over the charges of the dyons in a given subvolume. This is done by splitting the main simulation box in half along each of the three axes and computing the total charge in said half boxes. This results in three independent measurements per configuration, meaning the average of any power of Q is computed from 240,000 measurements. Figure 9 shows a typical distribution of Q values for a single temperature.

The temperature dependence of the topological susceptibility over the entire temperature range probed in this work is shown as blue points in Fig. 10. To make the comparison to lattice data easier, we show the *relative* susceptibility, with all sets to their values normalized just below the critical temperature. The issue of absolute comparison is further discussed in Appendix C.

FIG. 10. Dimensionless topological susceptibility as a function of temperature relative to the topological susceptibility just below T_c . The lattice data are taken from Refs. [29,32]. Lattice values are normalized relative to their stated $T = 0$ values. The data from Ref. [29] (green triangles) are the so-called two-smear data. The error bars on the dyon data are smaller than the point size.

With $\chi(T)$, like $\langle P(T) \rangle$, we see a clear first-order phase transition in the data. Unlike with the Polyakov loop, however, such an abrupt transition with a jump is not obvious from the lattice data points (although they, of course, do not contradict the existence of a jump). The topological observables have been analyzed on the lattice in many works, we compare our dyon results to those in Refs. [29,32], which cover a temperature range similar to what we have studied.

The (Euclidean) Lagrangians of generic $SU(N)$ gauge theories can be appended by an additional topological term

$$\mathcal{L} = \frac{1}{4} F_{\mu\nu}^a(x) F_{\mu\nu}^a(x) - i\theta q(x), \quad (21)$$

where θ is the so-called vacuum angle and $q(x)$ is the topological charge density as previously defined in Eq. (20). A nonzero θ explicitly breaks CP symmetry. In QCD it is known that $|\theta_{\text{QCD}}| \lesssim 10^{-10}$, as it is constrained by the upper bound on measurements of the neutron's electric dipole moment [33,34].

By expanding the free energy density $f(\theta)$ around $\theta = 0$, its dependence on θ can be studied at small, but nonzero, θ . It can be expanded as [35]

$$f(\theta) = f(0) + \frac{1}{2} \chi \theta^2 (1 + b_2 \theta^2 + b_4 \theta^4 + \dots), \quad (22)$$

where the coefficients b_n are related to cumulants of the topological charge *computed at* $\theta = 0$. We compute the first two terms, which are given explicitly by

$$b_2 = -\frac{\langle Q^4 \rangle - 3\langle Q^2 \rangle^2}{12\langle Q^2 \rangle},$$

$$b_4 = \frac{\langle Q^6 \rangle - 15\langle Q^2 \rangle\langle Q^4 \rangle + 30\langle Q^2 \rangle^3}{360\langle Q^2 \rangle}. \quad (23)$$

In the confined phase, we find that all b_2 values are consistent with b_2 being constant below T_c . These seven values vary around 0.02 – 0.03 and have an average $b_2(T < T_c) = 0.026$. Above T_c , b_2 quickly drops and then remains approximately constant just above 0.01.

This behavior disagrees with the available lattice data. The $T = 0$ value of b_2 has been particularly well studied on the lattice [36–38] with values of around $b_2(0) = -0.025$. On the high-temperature end, lattice data [32,39] find that b_2 approaches the value predicted by the dilute instanton gas approximation, $b_2(T) \rightarrow -1/12$.

Below T_c , as seen in Fig. 11, our values of b_2 are consistent with the magnitude of the $T = 0$ value predicted on the lattice, but with the opposite sign. In the high-temperature limit, we again see that our dyon model predicts positive values rather than negative, as well as being an order of magnitude smaller than the lattice results. Figure 9 shows a typical distribution; any non-Gaussianity is too small to be seen with the eye. Clearly, these small non-Gaussianities in the topological charge distribution are quite sensitive to the short-range dyon interactions. Changes to the dyon interactions should improve the agreement with lattice data.

FIG. 11. Expansion coefficient b_2 as a function of temperature.

Finally, our values for b_4 are compatible with zero for all temperatures, as is also observed on the lattice [36,40]. Upper limits from these lattice results constrain its value to $|b_4(T = 0)| < 10^{-3}$.

V. DYONS IN THE TRACE-DEFORMED GAUGE THEORY

A. Polyakov loop and the phase transition

Trace-deformed gauge theories (TDGT) were introduced in Refs. [24,41], adding certain terms containing powers of the Polyakov line to the theory action, such as

$$\Delta S_{\text{def}} = h \int d^3x |P(\vec{x})|^2, \quad (24)$$

with a new parameter h . At $T > T_c$, when in the undeformed theory the Polyakov loop is nonzero, the new term obtains an additional contribution and suppresses its value, shifting the theory back toward the confining holonomy. For large enough h the system returns to the $\langle P \rangle = 0$ phase, which we will call the “reconfined phase.”

These theories have been studied in numerous lattice simulations, of which we will mention those of the Pisa group [42–44]. Their main findings are that for a specific temperature above T_c at large enough $h > h_* \sim 1/3$, at which $\langle P \rangle$ returns to zero, there is no more dependence on h , and the reconfined phase is remarkably similar to the original (low-temperature) confined phase. It was shown to possess the same spectrum, topological observables, and even spectrum of periodic strings (torelons).

From the perspective of the instanton-dyon theory that we are developing, it is clear that the reconfined phase, like the confined one, corresponds to the symmetric value of the holonomy $\nu = 1/3$ and the same densities of all species L, M_1, M_2 of the dyons. Yet the temperature scale, and thus the periodicity interval of the Euclidean time τ , is different. Therefore, the absolute scale of the dyon action parameter $S_0 = 8\pi^2/g^2(T)$ must increase, making the system more dilute. And yet, the topological susceptibility χ is the same as at $T = 0$ despite a significantly reduced dyon density.

It is possible to study the instanton-dyon ensemble in a theory with arbitrary h by the addition of a deformation term to the free energy density $\Delta f_{\text{def}} = h\langle P \rangle^2$. Because this new term depends only on the value of the holonomy, one does not need to perform new MC simulations to study the effect of changing h ; one needs only to add the new term to the undeformed results and perform new fits to find the minima.

The first questions to ask are how does changing h affect the value of the Polyakov loop and at what value of h does the system become reconfined? Figure 12 shows the temperature dependence of the Polyakov loop for a few different values of h . As expected, the larger the trace deformation, the more suppressed the values of $\langle P \rangle$ become

FIG. 12. The value of the Polyakov loop as a function of temperature $\langle P(T) \rangle$ for different values of the trace-deformation parameter h .

at $T > T_c$. Additionally, we see that increasing h increases the critical temperature of the theory as well, as the Polyakov loop is suppressed back to the confining value.

The critical temperatures of the trace-deformed theories are determined via the same method as the original theory: the intersection of linear fits to f on both sides of the transition. At this point we are limited to determining T_c for $h \leq 40$, as above this value the Polyakov loop remains very close to the confining value and the minimum value of the holonomy fit becomes closer to $\nu = \frac{1}{3}$ than the holonomy step size used for the simulations, meaning that $\nu = \frac{1}{3}$ is compatible with our uncertainties for all temperatures studied. In order to accurately determine the critical temperature for large h , smaller steps in both S_0 and ν are necessary. This also makes determining the nature of the phase transition inconclusive at larger h . At small h , it is clear that the phase transition remains first order, while at larger h (above ~ 10) we do not have sufficient resolution in ν to determine whether the holonomy potential continues to have two distinct minima or becomes a smooth crossover.

While we are currently limited in how high of a critical temperature we can probe [up to $\sim 1.3T_c(0)$, per Fig. 13], the theory may have nontrivial behavior at higher temperatures. In the limit at which $T \rightarrow \infty$ the density of dyons goes to zero and only two terms in the free energy density remain: the (deconfinement-favoring) Gross-Pisarski-Yaffe potential and the (confinement-favoring) trace-deformation term. Clearly, which term dominates depends on the value of h . At $h > 5\pi^2/18 \simeq 2.74$ the confining holonomy is the global minimum.

FIG. 13. Critical temperature of the theory with trace-deformation parameter h relative to that of the pure Yang-Mills theory.

This leads to the conclusion that there are three distinct regimes of the TDGT:

- (i) $h < 5\pi^2/18$: The theory is confined at low temperatures and deconfined at high temperatures.
- (ii) $5\pi^2/18 < h < h_{\max}$: The theory is confined at low temperatures, deconfined in some intermediate region, and then *is confined again* at high temperatures.
- (iii) $h > h_{\max}$: The theory is confined at all temperatures.

While we cannot yet access high enough temperatures to directly see the second phase transition in regime (ii), the last value of $\langle P \rangle$ for $h = 40$ in Fig. 12 suggests that $\langle P \rangle$ may be starting to decrease and return to zero. This second phase transition and the three regimes of the theory have been observed on the lattice [41].

B. Topological observables of the reconfined theory

One of the most interesting features of the deformed gauge theory observed on the lattice [42–44] is that, when the trace deformation is large enough to return the system to the confining holonomy, the topological observables, namely, χ and b_2 , also return to the same values they had in the confined phase of the undeformed theory, and then show no more dependence on a further increasing h .

Rather than choose specific temperatures and vary h as was done in the lattice studies, we choose an arbitrarily large value of h and vary the temperature. As mentioned in the previous section, for some large value of h such that $h > h_{\max}$, the system should remain in the confined phase at all temperatures. In our dyon model, we can study this scenario, which we call the “maximally deformed” theory, by simply demanding that $\nu = \frac{1}{3}$ and determining the dyon densities that minimize the free energy density with this constraint. Because our individual simulations have the

FIG. 14. Dyon density of the maximally deformed theory as a function of temperature. Both dyon densities are equal ($n = n_M = n_L$).

fixed holonomy value $\nu = \frac{1}{3}$, $\langle P \rangle = 0$, the trace-deformation term does not contribute to the free energy density of these simulations and does not need to be considered in the fits.

The question then is whether or not the dyon ensemble, like the lattice theory, possesses the same topological observables in the maximally deformed theory as in the original confined phase. In the case of χ , our dyon model predicted not a constant value but an approximately linearly decreasing one. We observe analogous behavior to what is seen on the lattice; in the maximally deformed theory the abrupt jump in χ disappears and it displays the same temperature dependence above $T_c(0)$ as below. Comparing the dyon density (Fig. 14) and the topological susceptibility (Fig. 15), one can see that the decrease in χ is driven mostly by the decreasing dyon density. Although n_i decreases by a factor of ~ 4 (and the volume *increases* by the same factor), χ decreases by a factor of ~ 7 over the temperature range that we study. Per the definition $\chi = \langle Q^2 \rangle / \tilde{V}_4$ the value of $\langle Q^2 \rangle$ must decrease by a factor of ~ 2 , which we indeed to see.

The behavior of b_2 is more inconclusive (Fig. 16). It remains constant up to about $1.1T_c(0)$ and then decreases quickly and is compatible with zero at all temperatures above that point. Again, it remains positive at all temperatures. It should be noted that the error bars on the b_2 measurements are still quite large and the trend could look quite different with improved statistics.

In order to determine what drives this behavior, it is useful to look at some correlation functions in this deformed theory. It is clear that the ensemble has some

FIG. 15. Dimensionless topological susceptibility of the maximally deformed theory as a function of temperature. The error bars are smaller than the point size.

nontrivial temperature dependence even though it remains in the confined phase. The two main channels with positive correlation are, as in the undeformed theory, the $D\bar{D}$ channels and the instanton ($M_1 M_2 L$) channel. As the temperature is increased, the ensemble more strongly prefers pairing dyon and antidyons rather than the (anti-) instanton, as can be seen in Fig. 17. This is due to the

FIG. 16. Expansion parameter b_2 in the maximally deformed theory as a function of temperature.

FIG. 17. Spatial correlation functions of the dyons in the $M_1\bar{M}_1$ (left panel) and instanton (right panel) channels in the maximally deformed theory at three different temperatures.

increase in the strength of the $D\bar{D}$ classical attraction. Eventually, these pairing correlations grow strong enough to completely kill the correlation in the instanton channel.

In the original theory, the system prefers binding into instantons (M_1, M_2, L triplets) in the confined phase and then transitions into preferring $M_1\bar{M}_1$ and $M_2\bar{M}_2$ pairs at high temperatures; the density of $L\bar{L}$ is becoming small at this point. However, because the core sizes of the M_i dyons grow large, the binding in these channels does not become too large.

The maximally deformed theory then displays behavior not seen in the original theory. At high temperature the system becomes a three-component gas of $D\bar{D}$ pairs, with all types having equal densities and core sizes. Because the theory remains confined, the core sizes never become large and the correlation between dyons in $D\bar{D}$ pairs becomes very large. The topological observables are very sensitive to this binding, as the (anti)instantons and $D\bar{D}$ pairs have topological charges $Q = \pm 1$ and $Q = 0$, respectively. The shift toward the latter pairs leads to a *neutralization* of the topological charge and is responsible for the decrease in moments of the topological charge distribution, i.e., $\langle Q^2 \rangle$, $\langle Q^4 \rangle$, driving the values of χ and b_2 down at higher temperatures.

Looking to the future, one can see that this behavior has interesting implications when quarks are added to the theory. It is known that chiral symmetry restoration is directly related to the quark zero modes on the instantons. In particular, the quark interactions drive the system to form instanton–anti-instanton “molecules.” This neutralizes the fluctuations of the topological charge and shifts the Dirac eigenvalues away from zero at high temperatures, thereby restoring chiral symmetry [45]. In fact, in this work we have already observed $D\bar{D}$ pairing at higher temperatures.

We see here that such correlations continue to grow, even when the theory remains confined due to the deformation term in the action. This suggests that in the trace-deformed theory with quarks one may be able to see chiral symmetry restoration occur *inside* the confined phase.

VI. SUMMARY AND DISCUSSION

This paper has reported on the first direct numerical simulations of the ensemble of instanton dyons in the pure $SU(3)$ Yang-Mills theory. We have used classical and semiclassical one-loop measures which have derived the interdyon interactions. We have performed Monte Carlo simulations of an ensemble of dyons in a 3D cube with periodic boundary conditions over a range of temperatures, densities, and holonomy values.

Our main objective is to see whether the semiclassical ensemble of instanton dyons does or does not reproduce the deconfinement transition, which is, in this case, of the first order. We have indeed found that there are two distinct phases, the confined [with free energy minimal at holonomy value $1/3$; Fig. 3 (left panel)] and the deconfined [with free energy minimal elsewhere; Fig. 3 (right panel)]. We have been able to map out the holonomy potential, see explicitly the two nearly degenerate minima of the potential representing the transition between the two phases (red squares in Fig. 4), and study various properties near the critical temperature.

A comparison between our semiclassical model and lattice data for the VEV of the Polyakov loop $\langle P(T) \rangle$ is shown in Fig. 6. Remarkably, the jump of it at T_c is reproduced rather precisely, with some moderate deviations at higher temperatures. As shown in Fig. 7, this large jump results in L -dyon suppression in the deconfined phase,

while the density of M_i dyons has a rather smooth temperature dependence.

The pairwise spatial correlations between various dyons are shown in Fig. 8. Overall, they are in qualitative agreement with expectations. Note also that, for a system with a strong first-order transition, one does not see drastic changes in the correlations, except for an overall change of scale due to the change in the temperature.

We have studied fluctuations of the topological charge. Since each of our simulations has a fixed number of dyons, this is done by counting charges in the half box. A typical distribution is shown in Fig. 9, at first sight having just a normal Gaussian form. Its width (the topological susceptibility χ) is compared to the lattice data in Fig. 10. The magnitude of the jump and behavior in the deconfinement phase have been found to be quite similar, but the dependence at $T < T_c$ is somewhat different. Our results for non-Gaussianity parameter b_2 are perhaps still too noisy. Let us note that these observables, as well as the dyon correlations, are very sensitive to the details of the dyon interactions, particularly the short-range classical interactions, which are the strongest. These interactions are currently the most poorly understood aspect of the dyon model, with some parts being analytically derived (e.g., the Diakonov determinant) and others being simply phenomenological (e.g., the repulsive core). In order to achieve a quantitative agreement between the dyons and the lattice data, if possible, these interactions should be the subject of further study and improvement.

We have also reported on the first study of trace-deformed gauge theory in the instanton-dyon setting. As expected, by increasing the coupling h of the deformation term, one indeed suppresses the jump and value of the Polyakov loop in the deconfined phase. The phase transition location is also pushed to higher values; see Fig. 13. Overall, as on the lattice, we see that increasing h leads to a return to the topological susceptibility as in the confining phase of the undeformed theory. We still see, however, that this agreement is only partial; see, for example, the spatial correlations taken in the maximally deformed confining theory.

Completing this summary of our results, we again emphasize that the semiclassical model used, which has many orders of magnitude fewer degrees of freedom than lattice gauge theory, is able to explain properties of the deconfinement phase transition of the $SU(3)$ gauge theory quite well. Some quantities—like the jump in the Polyakov line—are reproduced precisely and others semiquantitatively, but we have not seen any serious disagreements. The double-trace deformation study also shows that both our model and the lattice react to this addition to the action in a very similar way.

Thinking of the future, the next step will, of course, be the inclusion of dynamical quark flavors via their zero modes and interactions. Such work will allow us to study not only the confinement (which will now be expected to be

a smooth crossover) but also the role of the dyons in chiral symmetry restoration.

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APPENDIX A: UNITS

Temperature is the main physical quantity of this work: it defines the holonomy, via $A_4^3 = 2\pi\nu T$, as well as the physical sizes of the dyons.

All parameters are presented as dependent on the instanton action S_0 , which is related to the temperature by

$$S_0 = \frac{8\pi^2}{g^2} = \left(\frac{11}{3} N_c - \frac{2}{3} N_f \right) \ln \left(\frac{T}{\Lambda} \right), \quad (\text{A1})$$

where, in pure $SU(3)$ gauge theory, $N_c = 3$ and $N_f = 0$.

As with previous work on the ensemble of $SU(2)$ dyons [16], the value of the parameter Λ is a choice that maps the instanton action S_0 to the temperature T . This parameter was chosen to be $\Lambda = 2.8$. It should be the subject of improvement in future comparisons with lattice data. The reader should keep in mind that this value is different than the one chosen for the previous $SU(2)$ studies, $\Lambda^{SU(2)} = 1.5$. Because the temperature scale is set by this choice, conversion to physical units may be done setting the dyons' critical temperature equal to that of the lattice gauge theory: $T_c = 9.82 \leftrightarrow 260$ MeV [46,47].

APPENDIX B: COMMENTS ON INTERACTION PARAMETERS AND FINITE-SIZE EFFECTS

1. Parameters of the dyon interactions

Let us take a moment to remind the reader that this is a *model* of the dyon ensemble. Certain parameters of the dyon interaction, namely, V_0 , x_0 , and M_D , are not known from first principles and are thus phenomenological parameters of the model. In the previous $SU(2)$ work [17] these parameters were chosen to be $(V_0, x_0, M_D) = (20, 2.0, 2.0)$. In the preliminary stages of testing of the $SU(3)$ model, it was found that these parameters were unsuitable for generating the desired phase transition. These parameters are sensitive to the details of the theory and one should not expect them to be identical for all N_c .

In this work, the parameters used were $(V_0, x_0, M_D) = (10, 4/3, 1.5)$. These parameters were chosen to produce a phase transition at around $S_0 \sim 12$, jumping from $\langle P \rangle = 0$ to $\langle P \rangle \simeq 0.4$. The choice of x_0 was not arbitrary, as when the factor of $1/\nu$ is included the dyons in the confined phase have the same dimensionless core radius as was used

in $SU(2)$. This choice of parameters exists on a 3D “island” in the parameter space in which such choices of the parameters possess reasonable properties. They can and should be further constrained by future data regarding identification of the dyons in lattice configurations. In particular, if dyon densities and correlations can be studied with sufficient statistics, such data can reveal details of the dyons’ interactions. Some correlations between dyons on the lattice (in physical QCD) can be found in Ref. [48], although the statistics are not yet sufficient to make such constraints.

Each of these parameters has a clear effect on the phase transition of the ensemble. Large values of any of these parameters favors the confined phase and drives T_c upward. In the case of V_0 and x_0 , large values make the repulsive cores larger, more strongly favoring the confining holonomy. A large value of M_D suppresses the long-range interactions, making the dyon cores comparatively more important. For a more systematic analysis of the effects of changing the parameters, see Ref. [17].

Additionally, the Debye mass is not necessarily a constant, but rather a temperature-dependent quantity $M_D(T)$. In fact, in the previous work by Larsen and Shuryak [16] the Debye mass was treated as an input parameter to be swept over, much like the densities, and only those configurations with input values consistent with its definition,

$$M_D^2 = \frac{g^2}{2V} \frac{\partial^2 F}{\partial \nu^2} \Big|_n, \quad (\text{B1})$$

were chosen. This increases the number of configurations to be tested but allows for a more general, temperature-dependent Debye mass. Both methods have been shown to produce reasonable properties for the $SU(2)$ dyon ensemble, so we have saved computational time by treating it solely as an input. One could also consider a more direct method in the future by simply taking the value of $M_D(T)$ as an input from the lattice data.

2. Finite-size effects

In principle, equilibrium statistical mechanics is derived in the thermodynamic limit $N_D, \tilde{V}_3 \rightarrow \infty$, which is not possible in numerical simulations. For such a finite numerical simulation, the main concern is whether the system size used is sufficiently large that the measured observables can be reliably extrapolated to the thermodynamical limit. The simplest way to check these effects is to simulate larger systems with the same parameters and study the dependence of some observables on the size N_D .

Here we discuss a representative example of the finite-size effects seen in Fig. 18. When one increases the size of the system by up to a factor of 2, there is a noticeable change in the free energy landscape. Looking at Eq. (9), there are only two terms which can vary with system size:

FIG. 18. Free energy density f as a function of dyon density with $S_0 = 12$, $\nu = \frac{1}{3}$ for three different system sizes.

the dyon interaction term Δf and the third term stemming from Stirling’s approximation, which has explicit $\tilde{V}_3$ dependence. Increasing the system size decreases the contribution from the third term as it goes to $1/\tilde{V}_3$. Subtracting this term from the results reveals that the contribution from the dyon interactions increases with system size. Both of these effects are reduced in the deconfined phase, where the density is lower.

The main factor in the finite-size effects regarding dyon interactions comes from dyons near the boundaries of the system. As long as a finite number of dyons and image boxes are used, there are dyons near the faces of the cube whose total short-range interactions are reduced. The fraction of dyons near the faces of the cube should scale as $N_D^{-1/3}$ and thus vanish in the thermodynamic limit. Parameters that determine the effective range of interactions such as the core sizes and Debye mass also play an important role in determining how quickly the results converge to the $N_D \rightarrow \infty$ limit.

Different quantities may converge at different speeds. In Fig. 18 it is seen that the value of the free energy minimum decreases by $\sim 2\%$ when one doubles the number of dyons. A simple linear fit of f as a function of $1/N_D$ gives an infinite-volume value of $f = -4.519$, a 4.5% decrease from the $N_D = 120$ value. The input parameters of the ensemble—the holonomy and densities—depend only on the *location* of the minimum, which clearly varies much less. Fitting the curves to quadratic forms gives the densities $n_M = 0.607, 0.609, 0.607$ for dyon numbers $N_D = 120, 180, 240$, respectively. These values agree within uncertainty and show no clear trend. Similar behavior was seen in the $SU(2)$ results of Lopez-Ruiz *et al.* [17],

who studied finite-volume effects in more detail and showed good results for a maximum ensemble size of $N_D = 88$. We conclude that the number of dyons $N_D = 120$ used in this work is sufficiently large to determine the thermodynamic properties of the dyon ensemble.

APPENDIX C: TOPOLOGICAL CHARGE FLUCTUATIONS

Here we present a general discussion of topological susceptibility measurements in our setting and on the lattice.

Suppose that a lattice of the 4-volume V_4 is used, and that instantons with an average density d_I populate it *randomly*. This leads to a Poisson distribution with a mean number $\langle n_I \rangle = d_I V_4$. The same is assumed for anti-instantons $\bar{I}$, and, as is well known, the susceptibility is simply the total density

$$\chi = \frac{\langle (n_I - n_{\bar{I}})^2 \rangle}{V_4} = d_I + d_{\bar{I}}. \quad (C1)$$

In instanton liquid simulations the numbers $N_I, N_{\bar{I}}$ are fixed, and fluctuations appear only if one uses the sub-box as proposed in Ref. [49] for studies of correlations in the instanton ensemble. Let the sub-box have a volume fraction $f \equiv v_4/V_4$. Thus, if dyons are also placed randomly, their distribution is binomial,

$$B(f, N, n) = \frac{N!}{n!(N-n)!} f^n (1-f)^{N-n}. \quad (C2)$$

In the limit when all volumes—and thus the numbers involved—are large, standard statistical mechanics textbook analysis leads to the conclusion that both Poisson and binomial distributions lead to Gaussian fluctuations around

their corresponding mean. Standard use of Stirling formula $\log(n!) = n \log(n/e)$ and $n = fN + \delta$ leads to

$$B(\delta) \sim \exp \left[-\frac{\delta^2}{2f(1-f)N} \right] \quad (C3)$$

or $\langle \delta^2 \rangle = f(1-f)N$. The topological susceptibility of the sub-box is then

$$\chi(f) = \frac{f(1-f)(N_I + N_{\bar{I}})}{fV_4} = (1-f)\chi_P, \quad (C4)$$

where χ_P is that for the unrestricted Poisson distribution defined above. Indeed, the fluctuation must vanish at $f \rightarrow 1$, but for small subsystem $f \rightarrow 0$ both become the same. Thus, in comparing the *absolute value* of the topological susceptibility that we measure to those on the lattice, one needs to multiply the former by $1/(1-f) = 2$.

Let us now calculate χ for randomly placed instanton dyons. Their total numbers in our setting are also fixed, and we always keep

$$N_L = N_{\bar{L}}, \quad N_{M1} = N_{\bar{M1}}, \quad N_{M2} = N_{\bar{M2}},$$

which ensures that the total magnetic and topological charges of the entire system are zero. The topological charge in the sub-box is

$$Q = (1-2\nu)(n_L - n_{\bar{L}}) + \nu(n_{M1} - n_{\bar{M1}}) + \nu(n_{M2} - n_{\bar{M2}}). \quad (C5)$$

It is an integer in two limiting cases, confining the holonomy $\nu = 1/3$ at $T < T_c$ and the trivial holonomy $\nu = 0$ at large T . The unrestricted topological susceptibility is then

$$\chi = \frac{((1-2\nu)^2(N_L + N_{\bar{L}}) + \nu^2(N_{M1} + N_{M2} + N_{\bar{M1}} + N_{\bar{M2}}))}{V_4}. \quad (C6)$$

In the confining case, with $\nu = 1/3$ and all dyon numbers equal to N_d , it is $6N_d/9V_4$. Comparing this to the case in which any triplet L, M_1, M_2 is tightly coupled into instantons with the same density $N_I = N_d$, one finds that

$$\chi(\text{random dyons}) = \frac{1}{3} \chi(\text{fully correlated dyons}). \quad (C7)$$

Indeed, the clustering of dyons into instantons increases the fluctuations. Conversely, the clustering of dyons into $D\bar{D}$ pairs (as indeed happens at higher temperatures) decreases the fluctuations.

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