Full $\mathcal{O}(a)$ improvement in electrostatic QCD

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Electrostatic QCD (EQCD) is a three-dimensional bosonic theory containing SU(3) and an adjoint scalar, which efficiently describes the infrared, nonperturbative sector of hot QCD and which is highly amenable to lattice study. We improve the matching between lattice and continuum EQCD by determining the final unknown coefficient in the $\mathcal{O}(a)$ matching, an additive scalar mass renormalization. We do this numerically by using the symmetry-breaking phase transition line of EQCD as a line of constant physics. This prepares the ground for a precision study of the transverse momentum diffusion coefficient $C(q_\perp)$ within this theory. As a by-product, we provide an updated version of the EQCD phase diagram.

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I. INTRODUCTION

At low energy scales, and therefore at low temperatures, the coupling of QCD becomes large and the theory's behavior becomes nonperturbative. Therefore we should not be surprised if perturbation theory does not work for thermodynamical or dynamical properties as one approaches the QCD crossover temperature, $T \sim 150$ MeV [1,2], from above. However, it came as a surprise just how badly perturbation theory works at scales up to many times the transition temperature. For instance, thermodynamical properties such as the pressure have an expansion in g , the strong coupling which is known up to $g^6 \ln(g)$ [3–8], and while the leading-order behavior is within 30% of the lattice result above 360 MeV [1,2], the series of corrections does not converge even for $T = 100$ GeV, a scale where perturbation theory should work well [9]. This problem was first understood broadly by Linde [10] and was diagnosed more completely starting in the mid-1990s with the work of Braaten and Nieto [11], who showed that the perturbative expansion could be understood as a two-step process. Treating the problem in Euclidean space, the time direction is periodic with period $\beta = 1/T$, corresponding in frequency space to a tower of discrete frequencies $\omega_n = 2\pi nT$, the Matsubara frequencies [fermions have $\omega_n = (2n + 1)\pi T$]. One can integrate out all but the $n = 0$ modes of the spatial gauge field A_i and its temporal

component A_0 : dimensional reduction [12,13]. This results in a three-dimensional (3D) theory of an SU(3) gauge field and an adjoint scalar (A_0 behaves as a scalar and we will call it Φ henceforth), which has been christened “3D electrostatic QCD” or EQCD for short.

Explicit loopwise-order calculations of the matching between full thermal QCD with quarks and EQCD [14,15] indicate that integrating out the nonzero Matsubara frequencies is a well-behaved perturbative procedure down to temperatures of order 300 MeV. It is the behavior of EQCD itself which is not under perturbative control. But one can solve EQCD nonperturbatively on the lattice, and this appears to generate much closer approximations to the full four-dimensional (4D) thermodynamics than perturbation theory alone [15–17].

EQCD is a 3D theory of bosons only, which is relatively easy to treat on the lattice; for most thermodynamical quantities, high-quality results were already available 20 years ago. But in 2008 Caron-Huot showed [18] that EQCD is also the right effective theory for computing a dynamical transport property, $C(q_\perp)$, the differential rate at which a highly relativistic colored particle exchanges transverse momentum with the medium [19,20]. This has important applications in hard particle suppression and jet modification in the hot QCD medium. For instance, the frequently discussed “transport coefficient” $\hat{q}$ is defined as the $q_\perp^2$ moment of $C(q_\perp)$, $\hat{q} = \int \frac{d^2 q_\perp}{(2\pi)^2} q_\perp^2 C(q_\perp)$. To calculate $C(q_\perp)$, one notes that its transverse-space Fourier dual $C(\mathbf{b}_\perp)$ is defined in terms of a Wilson loop with two spatial and two lightlike edges [20],

$$C(\mathbf{b}_\perp) = \lim_{L \rightarrow \infty} -\ln W[(0,0,0);(0,0,\mathbf{b}_\perp);(L,L,\mathbf{b}_\perp);(L,L,0)], \quad (1.1)$$

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where $W(a; b; c; d)$ is the (fundamental representation) Wilson loop connecting the four spacetime points $(a; b; c; d)$, and we have written $a = (a_t, a_z, \mathbf{a}_\perp)$. What Caron-Huot showed is that W can be replaced with a similar Wilson loop in EQCD, with the L -length edges replaced by a modified Wilson line which also incorporates the scalar field Φ , up to corrections which should be highly suppressed in any regime where dimensional reduction works. It would be extremely interesting to pursue a high-quality determination of $C(q_\perp)$ within EQCD, to extract *directly* important non-perturbative *dynamical* information about the behavior of hot QCD, of direct relevance for experiment.

Panero, Rummukainen, and Schäfer have made a first exploration of this quantity in EQCD [21]. However, it appears that the numerics are much more challenging than for standard thermodynamical quantities, especially for small $b_\perp$ values. Therefore it is essential to minimize lattice spacing errors, since the numerical cost of a study increases as approximately a^{-5} , with a the lattice spacing. In a 3D theory it should be possible to perform a lattice-continuum matching which is free of $\mathcal{O}(a)$ errors. Without doing so, the leading errors are of order $\mathcal{O}(a/b_\perp)$; with a -errors removed, the leading errors are $\mathcal{O}(a^2/b_\perp^2)$, a very significant improvement for small $b_\perp$. At the level of the Lagrangian parameters of EQCD, such an improvement was performed a long time ago [22]—*except* that one parameter remains undetermined at the $\mathcal{O}(a)$ level. When evaluating a particular composite operator such as the modified Wilson line, one must also determine the $\mathcal{O}(a)$ corrections to the operator; but this was done for the modified Wilson line operator a few years ago [23]. So we would have everything we need to proceed with a lattice study, free from any $\mathcal{O}(a)$ errors, if we only knew the lattice-continuum matching of that one remaining Lagrangian parameter. Specifically, while most Lagrangian terms receive $\mathcal{O}(a)$ corrections at one loop, the Φ -field mass-squared parameter receives (known) $\mathcal{O}(1/a)$ corrections at one loop and $\mathcal{O}(\ln(a))$, $\mathcal{O}(1)$ corrections at two loops [14]. The unknown $\mathcal{O}(a)$ errors arise at the three-loop level [23].

This paper will undertake the necessary technical development of determining this $\mathcal{O}(a)$ correction in the lattice-continuum matching of 3D EQCD theory. The direct diagrammatic evaluation appears too difficult to pursue; so we will use an alternative method to extract the corrections. Since the m_{3d}^2 -renormalization is the only missing $\mathcal{O}(a)$ -contribution, it can be determined by fitting to a line of constant physics. EQCD features a phase transition, which we will utilize to obtain such a line.¹

¹Note that the phase transition in EQCD is unphysical in the sense that it is not related to any phase transition in 4D thermal QCD. Indeed, 4D QCD with physical quark masses has a crossover at zero quark chemical potential [1,2]; the pure-gluon theory at high temperature has a Z_3 -breaking phase structure which is related to the EQCD phase transition in a one-loop analysis [14], but because EQCD lacks a true Z_3 symmetry, this is essentially a coincidence (see, however, Ref. [24]).

In the remainder of the paper, we present our investigation of the matching problem. Section II sets the theoretical stage. Section III presents our approach to determining the three-loop mass renormalization indirectly from lines of constant physics. We present our results in Sec. IV and leave conclusions and outlook to Sec. V. A few odds and ends appear in two Appendixes.

For the impatient reader, here is a very short summary. The theory EQCD has two parameters, the mass-squared y and scalar self-coupling x (the gauge coupling just sets a scale). For a given value of the self-coupling x , there is a critical y -value where a phase transition occurs. We find this point at several lattice spacings, and extrapolate to the continuum behavior; the slope of the fit at $a = 0$ is precisely the $\mathcal{O}(a)$ mass correction which must be compensated. Perturbative arguments show that the resulting slope should depend on x as a third-order polynomial. Determining this at several x -values allows us to fit all polynomial coefficients, which are presented with their covariance matrix in Eq. (4.4) and Table III.

II. THEORETICAL SETUP

The theory EQCD is a three-dimensional $SU(3)$ gauge theory with gauge field $A_i^a T^a$ ($i = 1, 2, 3$ and $a = 1 \cdots 8$) with a real adjoint scalar field Φ which can be understood as the dimensional reduction of the 4D Euclidean A_0 field component. The continuum action is

$$S_{\text{EQCD,c}} = \int d^3x \left(\frac{1}{2g_{3d}^2} \text{Tr} F^{ij} F^{ij} + \text{Tr} D^i \Phi D^i \Phi + m_D^2 \text{Tr} \Phi^2 + \lambda (\text{Tr} \Phi^2)^2 \right). \quad (2.1)$$

The parameter m_D^2 has logarithmic scale dependence which we resolve in the same way as in [14]. We will use the coupling g_{3d}^2 , which has dimensions of energy, to set the scale, and we work in terms of the dimensionless ratios $x \equiv \lambda/g_{3d}^2$ and $y \equiv m_D^2(\bar{\mu} = g_{3d}^2)/g_{3d}^4$, originally introduced by [14,25].

We will not present the full details of our lattice implementation or update algorithms, since they are almost identical to [26]. We use the standard Wilson gauge action and nearest-neighbor scalar gradient or “hopping” term. The only crucial difference to the presented $SU(2) +$ fundamental scalar-case concerns the treatment of the hopping term in the gauge field update. It arises from the scalar kinetic term, which translates into

$$\begin{aligned} & \int d^3x \text{Tr} D^i \Phi D^i \Phi \\ & \rightarrow 2Z_\Phi \sum_{x,i} \text{Tr} \left[\Phi_L^2(x) - \Phi_L(x) U_i(x) \Phi_L(x + a\hat{i}) U_i^\dagger(x) \right] \end{aligned} \quad (2.2)$$

in the lattice formulation, where Φ_L is the rescaled, dimensionless lattice version of the adjoint scalar field, Z_Φ is a field renormalization factor, and $U_i(\mathbf{x})$ is the standard gauge link at lattice site $\mathbf{x}$ in direction i . In contrast to the fundamental scalar case treated in [26], the present hopping term is nonlinear in the link. Therefore, it has to be incorporated into the link update via a Metropolis step. Our scalar update, on the other hand, is a mixture of heat-bath updates with the $x\text{Tr}\Phi^4$ term included by Metropolis accept/reject and the overrelaxation update introduced in Ref. [26]. We update sites in checkerboard order. Our code was modified from the OPENQCD-1.6 package [27].

Now we return to the parameters of the continuum and lattice actions. For this choice of parameters, one-loop relations between the lattice gauge and scalar couplings and their continuum values, and two-loop relations for the scalar mass, are known; we use the expressions from [23].² The matching between the lattice and continuum is such that we know the lattice x and g_{3d}^2 parameters up to $\mathcal{O}(a^2 g_{3d}^4)$ corrections. Effects from higher-dimension operators (present in the Wilson action and nearest-neighbor hopping term) are also of $\mathcal{O}(a^2)$. We also know the multiplicative rescaling between y and y_{latt} to the same precision, and we know the $\mathcal{O}(1/a)$ and $\mathcal{O}(1, \ln(a))$ additive contributions to y . Only the (three-loop) $\mathcal{O}(a)$ additive contribution to y is unknown. Therefore any $\mathcal{O}(a)$ difference in a physical result between lattice treatments at different lattice spacings must arise due to this additive contribution.

The phase structure of EQCD was extensively examined in the 1990s, e.g., in [28]. The theory has a $\mathbb{Z}_3$ symmetry which is broken if $\text{Tr}\Phi^3$ takes a nonvanishing value. There is a line of phase transitions separating a large- y region, where $\mathbb{Z}_3$ symmetry is preserved, from a small- y region where $\mathbb{Z}_3$ symmetry is spontaneously broken. Unlike the transition in $SU(2)$ fundamental [26] or adjoint [14] theories, this transition line extends over all x values, since the phases are distinguished by a global discrete symmetry breaking. At small x values the transition is first order; there is a tricritical point, and for large x values it is second order [28]. Values of x corresponding to dimensional reduction from physical temperatures and quark numbers all land in a region where the transition is first order; they also lie below the critical value y_{crit} , so physical QCD corresponds to metastable points in the EQCD phase diagram. (We emphasize again that the phase transition in EQCD is not

related to any thermal phase transitions which may or may not occur in 4D QCD.)

Our methodology will consist of determining, for a given x value, the value y_{crit} where the phase transition occurs. Doing so at a series of lattice spacings provides a lattice determination of the lattice spacing a dependence of y_{crit} . Since the only $\mathcal{O}(a)$ error remaining in our lattice implementation of the theory is an additive shift to y , the slope of $y_{\text{crit}}(a)$ when we extrapolate the lattice spacing $a \rightarrow 0$ determines the unknown linear-in- a correction to y at each given x value.

Formally, we know that the $\mathcal{O}(a)$ lattice-continuum additive δy contribution arises from three-loop scalar self-energy diagrams in lattice perturbation theory [22]. Even without computing these graphs, we can see that they involve 0, 1, 2, and 3 factors of the scalar self-coupling. Therefore, making $N = 3$ in the expression from [23] explicit, we give the lattice mass squared in terms of the continuum y value,

$$S_{\text{EQCD,L}} = \cdots + \sum_x Z_2(y + \delta y) \text{Tr}\Phi_L^2, \quad (2.3)$$

$$Z_2 = g_{3d}^4 a^2 \left(1 + g_{3d}^2 a \left[-\frac{\Sigma}{8\pi} + (-9 + 10x) \frac{\xi}{4\pi} \right] \right), \quad (2.4)$$

$$\begin{aligned} \delta y = & -\frac{1}{g_{3d}^2 a} \frac{\Sigma}{4\pi} (6 + 10x) + \delta y_{3\text{loop}} \\ & -\frac{1}{16\pi^2} \left[10x \left(\frac{3}{2} \Sigma^2 + 3\Sigma\xi - 6\delta \right) \right. \\ & + \left(\ln \left(\frac{6}{g_{3d}^2 a} \right) + \zeta - 3\Sigma\xi \right) (60x - 20x^2) \\ & \left. + 9 \left(\frac{7}{8} \Sigma^2 - \frac{\Sigma\pi}{6} + \frac{31\Sigma\xi}{6} + 2\kappa_1 - \kappa_4 + 4\rho - 4\delta \right) \right], \quad (2.5) \end{aligned}$$

where $\zeta = 0.08849$, $\delta = 1.942130$, and $4\rho - 2\kappa_1 + \kappa_4 = -1.968325$. The undetermined $\mathcal{O}(a)$ additive contribution must be parametrically of the form

$$\delta y_{3\text{loop}} = g_{3d}^2 a (C_0 + C_1 x + C_2 x^2 + C_3 x^3). \quad (2.6)$$

With results at enough x values, we can perform a polynomial fit to extract these coefficients and use it to determine the correction at any x value.

Eventually we want to apply EQCD to study QCD. Dimensional reduction at a specific temperature (hence gauge coupling) and number of light fermions leads to a specific x and y value. The two-loop reduction formulas between high-temperature (3 + 1)-dimensional full QCD and EQCD were worked out by Kajantie *et al.* [14,15], and we use a nonperturbative value of $\Lambda_{\overline{\text{MS}}}$ from [29]. These lead to the specific x and y values, which we will later investigate for $C(q_\perp)$ behavior, shown in Table I. To minimize errors in a future investigation, we will examine

²The paper is written for general gauge groups, where there are two independent scalar self-couplings. These are equivalent in $SU(3)$, so we take $x_2 = 0$ in their notation. Note that in the lattice action in [23], x_1 and x_2 actually have to be interchanged for consistency with the rest of that paper. Also, since the normalization of the lattice scalar field is arbitrary, we have chosen $Z_\Phi = 1$; that is, we normalize our hopping term to have a unit norm.

TABLE I. Three-dimensional EQCD parameters for four typical scenarios.

T	n_f	x	y
250 MeV	3	0.08896	0.452423
500 MeV	3	0.0677528	0.586204
1 GeV	4	0.0463597	0.823449
100 GeV	5	0.0178626	1.64668

the mass renormalization at the x -values indicated, except the smallest value where our method will prove ineffective. We will also study larger values of x which do not correspond to any physical QCD regime.

The determination of y_{crit} faces the usual challenges of supercritical slowing down, associated with determining a first-order phase transition point numerically. In the next section we present a methodology for evading this problem.

III. OUR METHOD

The standard way of determining y_{crit} would be by applying multicanonical reweighting in order to enforce tunneling between the two phases [28]. This is rather inefficient, so we develop another approach to efficiently determine the transition temperature of a first-order phase transition on the lattice.

The main idea is to prepare a lattice configuration where the two phases coexist and are permanently compared to each other at the phase boundaries. If we miraculously guessed the exact value of y_{crit} , the symmetric phase volume would change only via Brownian motion. If our value for y were close to but not exactly y_{crit} , the phase boundaries would feel a small net pressure and would tend to allow the preferred phase to expand at the expense of the other. This leaves us with two questions:

- (i) How do we prepare such configurations?
- (ii) How can we tune the mass to its critical value and balance the Brownian motion of the phase boundaries?

The true order parameter of EQCD is $\text{Tr}\Phi^3$, which indicates whether the $\mathbb{Z}_3$ -symmetry of Φ is present or broken. However, the phase transition can also be spotted in $\text{Tr}\Phi^2$ (see Fig. 1), which has smaller fluctuations and leads to a more stable phase discriminator; so we use it in the following. Our approach begins by bounding y_{crit} by performing a simulation in a modest-sized cubic box, starting from a quite positive y value and decreasing it after each update sweep. At some value, $\text{Tr}\Phi^2$ abruptly jumps. Then one steadily increases y until the value abruptly falls. This determines upper and lower *spinodal* y -values; y_{crit} must lie between, typically close to the upper value.

Next we estimate $\text{Tr}\Phi_{\text{symm}}^2$ and $\text{Tr}\Phi_{\text{brok}}^2$, the values of $\text{Tr}\Phi_L^2$ in each of these phases at a mass close to the transition temperature, which we do in separate simulations which are initialized with either vanishing or large constant Φ values. The method will be rather insensitive to the exact values of these quantities, so it is not important if the determinations are from somewhat incorrect y values.

Next we set up our mass tuning algorithm. We work in a rectangular periodic lattice with one long (L_z) direction and two equal shorter ($L_x = L_y$) directions. Initially we make the y (Lagrangian) value z -coordinate dependent,

$$y(z) = y_{\text{crit,est}} + \Delta y \cos(2\pi z/L_z), \quad (3.1)$$

with Δy chosen initially to be large enough that $y_{\text{crit,est}} \pm \Delta y$ are above/below the spinodal values. After a series of update sweeps, the field will find the symmetric phase where y is large and the broken phase where y is small, generating our configuration with both phases and two

FIG. 1. $\text{Tr}\Phi^3$ and $\text{Tr}\Phi^2$, integrated over transverse directions, as a function of the z direction in a $36^3 \times 96$ box at $g_{3d}^2 a = \frac{1}{3}$, $x = 0.08896$, and $y = 0.47232$. There is a region near 0 (periodically identified with 96) which is in the symmetric phase, and a region near 50 which is in the broken phase, as well as two phase boundaries. The phases are visible in either order parameter but the fluctuations in $\text{Tr}\Phi^2$ are smaller.

phase boundaries. Then the magnitude of Δy is gradually lowered over a series of update sweeps; if one phase starts to win out over the other, the estimated critical value is adjusted.

With our starting two-phase configuration and estimated y_{crit} in hand, we proceed to the more accurate determination of y_{crit} . We continue to evolve with a space-uniform y value, but we adjust it after each lattice site update according to

$$y_{L,\text{new}} = y_{L,\text{old}} + c_B \cdot \left(\frac{\frac{1}{V} \sum_x \text{Tr} \Phi^2 - \text{Tr} \Phi_{\text{symm}}^2}{\text{Tr} \Phi_{\text{brok}}^2 - \text{Tr} \Phi_{\text{symm}}^2} - 0.5 \right), \quad (3.2)$$

where $y_L \equiv Z_3(y + \delta y_{2\text{loop}})$ and c_B is a small coefficient that controls the strength of the adjustment. The quantity in brackets here is an estimate for the fraction of the volume which lies in the broken phase, based on the known (approximate) values of $\text{Tr} \Phi^2$ in each phase. Therefore, the adjustment term shifts y upwards (making the symmetric phase more preferred) when more volume is in the broken phase and downwards (making the broken phase more preferred) if more of the volume is symmetric.

The coefficient c_B is small, $\mathcal{O}(\frac{1}{N_x N_y N_z})$, such that the evolution of y is as mild as possible, consistent with enough restorative force to prevent either phase from “winning.” Specifically, whenever y deviates from y_{crit} , there is a net force on the interface, equal to the surface area times ΔF , the free energy difference between phases. At $y = y_{\text{crit}}$, $\Delta F = 0$, and there is no net force on the interface. Away from $y = y_{\text{crit}}$, we can expand ΔF in a Taylor series in $y - y_{\text{crit}}$. At leading order in small $y - y_{\text{crit}}$, the free energy difference will be linear in $y - y_{\text{crit}}$, and the central value of y which maintains coexistence will equal y_{crit} . At quadratic order, $d^2 F / dy^2 \neq 0$ means that the restorative force is slightly biased, and we will obtain an incorrect value for y_{crit} . We test for such a distortion by performing a second evolution where c_B is twice as large, to confirm that the central value of y is the same within errors (which it is in all cases we considered).

IV. RESULTS

We use the procedure described in the previous section to determine the critical value $y_{\text{crit}}(x, a)$ for several values of the scalar self-coupling x , each at several lattice spacings. The exact list of lattices considered is given in Table V. Because our procedure leads to relatively long autocorrelation in the estimated y_{crit} value, the errors must be determined via the jackknife method using relatively wide jackknife bins; we vary the bin widths until the error estimates stabilize. We then subtract the known one- and two-loop contributions and apply the known multiplicative rescalings [22] from the results and convert $y_{L,\text{crit}} \rightarrow y_{2\text{loop,crit}}$. For each x value, we must extrapolate this quantity to zero lattice spacing; the intercept is the

TABLE II. Results of our five EQCD simulation sets.

x	$y_{\text{crit,cont}}$	$\delta y_{3\text{loop}} / g_{3d}^2 a$
0.0463596	0.9293(13)	-0.467(19)
0.0677528	0.67627(85)	-0.298(10)
0.08896	0.54092(76)	-0.1750(74)
0.13	0.4043(18)	-0.037(18)
0.2	0.2961(15)	0.004(15)

continuum critical y value, and the slope at the intercept is the desired $\mathcal{O}(a)$ additive correction to the scalar mass.

Because our $y_{\text{crit}}(x, a)$ results are quite precise but the a values are not extremely small, we anticipate that $y_{\text{crit}}(x, a)$ contains corrections beyond linear order in a . In principle, we could straightforwardly fit a polynomial of order N_{poly} in $g_{3d}^2 a$ as

$$y_{\text{crit}}(g_{3d}^2 a) = \sum_{j=0}^{N_{\text{poly}}} y_j (g_{3d}^2 a)^j. \quad (4.1)$$

However, as often occurs, ever-higher-order coefficients are ever less certain, and including too many coefficients tends to overfit the data and artificially inflates the final fitting errors. In order to extract these coefficients as efficiently as possible from the data, we would like to build in our knowledge about the convergence of the perturbative series to the fit. A useful tool to implement this is constrained curve fitting [30,31]. Motivated by a rough estimate of the radius of convergence $(g_{3d}^2 a)_{\text{conv}} \approx 0.5$, we make the *a priori* guess

$$|y_i| \leq \frac{y_0}{2^i}, \quad (4.2)$$

having obtained y_0 from a standard, unconstrained fit. We then use this estimate to choose the size of a zero-centered chi square prior on each fitting parameter. The procedure has almost no impact on the determined values of y_0 and y_1 , where the data are far more constraining than the priors. In practice, a quadratic polynomial is sufficient to give a good fit with a reasonable χ^2 . The results of these fits are given in Table II, and the fits themselves are displayed in Fig. 2. We also confirmed by varying the volume that any finite-volume effects are smaller than our statistical error bars.

We caution the reader that, while y_0 and y_1 can be interpreted as the continuum critical point and the three-loop $\mathcal{O}(a)$ additive mass renormalization coefficient, we cannot interpret y_2 as a four-loop mass renormalization or use it to further improve the lattice-continuum matching. That is because there are many uncontrolled $\mathcal{O}(a^2)$ corrections which influence y_2 . For instance, there are unknown two-loop $\mathcal{O}(a^2)$ lattice-continuum corrections to x , which influence the critical value via $(dy_{\text{crit}}/dx)\delta x$. Similarly, tree-level $\mathcal{O}(a^2)$ high-dimension operators and

FIG. 2. Fits of $\mathcal{O}(g_{3d}^2 a)$ behavior for different x .

$\mathcal{O}(a^2)$ corrections to g^2 (which we could interpret as uncertainties in the scale setting) also lead to $\mathcal{O}(a^2)$ effects in the y_{crit} value. Because $(dy_{\text{crit}}/dx) \sim x^{-2}$, the $\mathcal{O}(a^2)$ and other higher-order effects will become severe as we go toward small x values. Therefore small x requires the use of very fine lattices. Furthermore, when x is small, there becomes a hierarchy of mass scales in the problem: $m_{A,\text{brok}} \gg m_\Phi \gg m_{A,\text{symm}}$. Both effects make the accurate extraction of y_1 at small x very numerically demanding. Therefore we did not treat the smallest x value shown in Table I. Instead, we add two larger values of x , $x = 0.13$ and $x = 0.20$, which are still within the domain where the transition is first order, but which give us a broader x range over which to fit y_1 as a function of x .

FIG. 3. Grand fit of $\frac{\delta y_{3\text{loop}}}{g_{3d}^2 a}(x)$ with error band.

TABLE III. Covariance matrix of the grand fit.

$\text{cov}(C_i, C_j)$	C_0	C_1	C_2	C_3
C_0	0.001700	-0.02997	0.1101	-3.563×10^{-8}
C_1	-0.02997	0.5451	-2.046	1.129×10^{-6}
C_2	0.1101	-2.046	7.899	-1.079×10^{-5}
C_3	-3.563×10^{-8}	1.129×10^{-6}	-1.079×10^{-5}	3.025×10^{-5}

Next we use our results for $y_1(x)$ to fit its overall x dependence. The parametric form of the $\mathcal{O}(g_{3d}^2 a)$ -correction [23] was given in (2.6). The x^3 coefficient corresponds to three-loop diagrams containing only scalar lines. It is therefore equal to the $\mathcal{O}(a)$ mass renormalization term in the theory in the $g_{3d}^2 \rightarrow 0$ limit, which is a scalar theory. We explain our (different) procedure to treat this scalar theory in Appendix A; our analysis leads to the result

$$C_3 = \frac{\delta \tilde{y}_{3\text{loop}}}{\lambda a} = 0.0151(55). \quad (4.3)$$

Here $\tilde{y} \equiv m^2(\mu = \lambda)/\lambda^2$ is the scalar mass, made dimensionless using the scale λ rather than the scale g_{3d}^2 ; it equals y/x^2 up to the effect of the different renormalization scale. We incorporate this result as a prior in fitting a cubic polynomial to the results of Table II. The resulting fit,

$$\begin{aligned} \frac{\delta y_{3\text{loop}}}{g_{3d}^2 a}(x) &= 0.0151(55)x^3 - 31.8(28)x^2 \\ &+ 10.80(74)x - 0.886(41), \end{aligned} \quad (4.4)$$

is displayed in Fig. 3. We report the full error covariance matrix in Table III. This fit constitutes our main result.

As a corollary, we provide an updated version of the EQCD phase diagram. The version from [28] does not include continuum-extrapolated critical masses. The intercept of our

EQCD fits delivers these critical masses. Additionally, the $x \rightarrow 0$ limit

$$xy_{\text{crit}} = \frac{3}{8\pi^2} \quad (4.5)$$

is known perturbatively [28]. We present our data, and this limiting value, in Fig. 4. In addition, to guide the eye,³ we include a cubic fit of xy_{crit} as a function of x , displayed by a dashed line. There is quantitative agreement with the phase diagram in [28] at small x , but at large x we find that the prominent bending down of the xy_{crit} curve found by [28] arose because they failed to take a continuum limit.

Kajantie *et al.* [28] found that the tricritical point occurs at $x = 0.25$, beyond which the phase transition becomes of second order. We have not studied x values larger than $x = 0.2$, so we cannot make any statement about the location of the tricritical point.

As a by-product our study also produces values for the discontinuity in $\text{Tr}\Phi^2$ across the phase transition point and for the $\mathcal{O}(a)$ additive correction to the $\text{Tr}\Phi^2$ operator, which was also not previously known. We postpone these secondary results to Appendix B.

V. CONCLUSION AND OUTLOOK

We have computed the remaining $\mathcal{O}(a)$ improvement coefficient in the lattice-continuum matching of 3D EQCD [SU(3) gauge theory with an adjoint scalar in three space dimensions]. We did so by using the first-order phase transition point as a fixed physical point. We developed a new methodology to efficiently extract the critical scalar mass where the first-order transition occurs. Determining the critical scalar mass $y_{\text{crit}}(x, a)$ as a function of a for fixed x allows an extrapolation to the continuum limit; the linear term in the extrapolation is the desired improvement coefficient. We then performed a grand fit to its known functional form. As a by-product, a continuum-extrapolated update of the EQCD phase diagram was obtained.

Now that we are in possession of the last missing ingredient, we aim to compute the modified EQCD-Wilson loop that leads to $C(q_\perp)$ and extrapolate it to the continuum. The continuum extrapolation is drastically

FIG. 4. Updated version of the phase diagram of EQCD. The phase below the data points is the $\mathbb{Z}_3$ -broken phase, and the one above is $\mathbb{Z}_3$ -symmetric. The dashed line is a fit to the data points, to help guide the eye.

³In fact, we expect nonanalytical behavior as $x \rightarrow 0$, due for instance to the two-loop $\Phi^2 \ln(\Phi^2/\mu)$ terms in the effective potential [32] which give rise to $xy_{\text{crit}} - 3/8\pi^2 \sim x \ln(x)$ corrections to Eq. (4.5).

facilitated by our completion of the renormalization [21]. The jet broadening coefficient $\hat{q}$ can be derived as the second moment of $C(q_\perp)$. We hope that the resulting nonperturbative information on $C(q_\perp)$ will be of utility in studying and interpreting the jet modification arising from the hot QCD medium in relativistic heavy ion collisions.

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TABLE IV. Simulation parameters for the pure scalar simulation.

λa	$N_x N_y N_z$	Total statistics
1/2	16^3	402900
1/3	24^3	1490120
1/4	32^3	2487440
1/6	48^3	2931750
1/8	64^3	2513280

TABLE V. Parameters and results of EQCD simulations.

$g_{3d}^2 a$	x_{cont}	$N_x N_y N_z$	$y_{\text{crit,cont}}$	Statistics y_{crit}	$\text{Tr}\Phi_{\text{brok}}^2/g_{3d}^2$	$\text{Tr}\Phi_{\text{symm}}^2/g_{3d}^2$
1/6	0.0463597	$72^2 \times 192$	0.824773(45)	300690	14.0477(40)	-0.22234(28)
1/8	0.0463597	$96^2 \times 256$	0.855935(85)	373030	15.4237(89)	-0.23064(43)
1/12	0.0463597	$144^2 \times 384$	0.88387(28)	37170	17.716(12)	-0.23390(77)
1/16	0.0463597	$192^2 \times 512$	0.89504(62)	1300	17.714(14)	-0.23748(74)
1/24	0.0463597	$192^2 \times 512$	0.9072(21)	1430	17.585(57)	-0.2355(17) ^a
1/4	0.0677528	$48^2 \times 128$	0.59100(19)	13110	6.7502(59)	-0.11392(62)
1/6	0.0677528	$72^2 \times 192$	0.62149(12)	150000	7.6155(72)	-0.12043(55)
1/8	0.0677528	$96^2 \times 256$	0.63661(11)	200000	7.960(14)	-0.12101(78)
1/12	0.0677528	$144^2 \times 384$	0.64963(29)	38990	8.287(15)	-0.12400(80)
1/16	0.0677528	$192^2 \times 512$	0.6546(11)	1910	8.4103(61)	-0.1228(12)
1/3	0.08896	$36^2 \times 96$	0.47232(24)	10000	4.0728(22)	-0.03277(47)
1/4	0.08896	$48^2 \times 128$	0.49119(14)	100000	4.4343(53)	-0.03489(59)
1/6	0.08896	$72^2 \times 192$	0.50940(15)	150000	4.7728(35)	-0.0344(10)
1/8	0.08896	$96^2 \times 256$	0.51736(20)	97500	4.9249(58)	-0.0336(11)
1/12	0.08896	$144^2 \times 384$	0.52565(45)	44530	5.052(10)	-0.0321(13)
1/3	0.13	$36^2 \times 96$	0.37184(94)	10000	2.3337(64)	0.1112(15)
1/4	0.13	$48^2 \times 128$	0.38341(83)	100000	2.3899(64)	0.1126(19)
1/6	0.13	$72^2 \times 192$	0.39323(21)	150000	2.4703(75)	0.1190(38)
1/8	0.13	$96^2 \times 256$	0.39702(31)	109230	2.5371(82)	0.1246(39)
1/12	0.13	$144^2 \times 384$	0.3982(11)	120600	2.618(13)	0.1332(65)
1/3	0.2	$36^2 \times 96$	0.27743(41)	12340	1.3115(74)	0.578(32)
1/4	0.2	$48^2 \times 128$	0.28595(34)	21030	1.283(13)	0.630(34)
1/6	0.2	$72^2 \times 192$	0.29214(37)	66160	1.2850(81)	0.650(24)
1/8	0.2	$96^2 \times 256$	0.29377(48)	122080	1.323(11)	0.713(37)
1/12	0.2	$144^2 \times 384$	0.29393(97)	3330	1.390(14)	0.707(26)

^aFor the sake of feasibility, we did not scale the volume here, accordingly. However, Ref. [34] states that no finite volume effects occur for $\beta = \frac{6}{g_{3d}^2 a}$ being smaller than the smallest extent of the lattice.

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APPENDIX A: ALGORITHM FOR PURE SCALAR CASE

The large- x limit of EQCD is the same as the $g_{3d}^2 \rightarrow 0$ limit (provided we work in terms of $\tilde{y} \equiv y/x^2 = m^2/\lambda^2$ and track the lattice spacing in terms of $\lambda a = g_{3d}^2 a x$). In this limit, we have an 8 (real) component scalar theory with an $\mathcal{O}(8)$ symmetry and a second-order phase transition where this symmetry is spontaneously broken to $\mathcal{O}(7)$. The x^3 term in the scalar mass renormalization of EQCD arises purely from scalar diagrams which are identical to those in this theory; therefore we can determine this coefficient by studying the $\mathcal{O}(\lambda a)$ corrections to $\tilde{y}$ in this scalar field theory.

A natural approach would be to use, as a line of constant physics, the second-order phase transition point. However, this would face the usual problems of critical slowing down and the inaccuracy of establishing the exact transition point. So we choose instead to compare $\tilde{y}$ between different lattice spacings by finding the *pseudocritical* value where the theory in a specific physical volume encounters a specific

FIG. 5. Continuum extrapolation of $\frac{\Delta \text{Tr} \Phi^2}{g_{3d}^2}$, the difference of the broken and symmetric phase values of $\frac{\text{Tr} \Phi^2}{g_{3d}^2}$, at different x . The intercept in (f) was determined analytically in [28] and was incorporated into that plot.

pseudocritical criterion. We choose the volume to be $\lambda L = 8$ and select as the pseudocritical condition that the fourth-order Binder cumulant [33]

$$\mathcal{B} \equiv \frac{\langle (\text{Tr} \bar{\Phi}^2)^2 \rangle}{\langle \text{Tr} \bar{\Phi}^2 \rangle^2}, \quad (\text{A1})$$

where $\bar{\Phi} \equiv \frac{1}{N^3} \sum_x \Phi_L(x)$, takes the value $\mathcal{B}_{\text{pc}} = 1.073$. Because the Binder cumulant is dominated by infrared physics and is insensitive to the lattice spacing up to subleading corrections and renormalization effects (which are what we want to study), this should occur at the same *physical* y value at every lattice spacing up to $\mathcal{O}(a^2)$ or

higher corrections. Our set of simulation parameters can be found in Table IV. The results already appeared in the last panel of Fig. 2.

APPENDIX B: EQCD SIMULATION PARAMETERS AND PHASE TRANSITION PROPERTIES

1. Parameters and table

In Table V, we provide parameters and direct results of our EQCD simulations as well as values for $\text{Tr} \Phi^2$ in both

FIG. 6. Fits of the symmetric phase value of $\frac{\text{Tr} \Phi^2}{g_{3d}^2}(g_{3d}^2 a)$ at different x and grand fit.

TABLE VI. Continuum-extrapolated $\frac{\text{Tr}\Phi^2}{g_{3d}^2}$ in the symmetric phase at criticality, $\mathcal{O}(a)$ operator improvement of $\frac{\text{Tr}\Phi^2}{g_{3d}^2}$, and continuum-extrapolated difference of $\frac{\text{Tr}\Phi^2}{g_{3d}^2}$ in the two phases at criticality.

x	$\text{Tr}\Phi_{\text{symm,cont}}^2/g_{3d}^2$	$\delta\text{Tr}\Phi_{3\text{loop}}^2/g_{3d}^4 a$	$\Delta\text{Tr}\Phi_{\text{cont}}^2/g_{3d}^2$
0.0463597	-0.2350(24)	-0.081(44)	18.232(27)
0.0677528	-0.1231(22)	-0.019(30)	8.692(13)
0.08896	-0.0272(27)	-0.072(25)	5.177(11)
0.13	0.151(11)	-0.256(70)	2.502(24)
0.2	0.763(76)	-0.66(85)	0.689(33)

phases at criticality. We converted $\text{Tr}\Phi_{\text{L,crit}}^2 \rightarrow \frac{\text{Tr}\Phi_{\text{crit,cont}}^2}{g_{3d}^2}$, where we display the latter in the table, via all known contributions up to $\mathcal{O}(g_{3d}^2 a)$ in Eq. (B3) [22]. For the sake of readability, we will refer to $\frac{\text{Tr}\Phi_{\text{crit,cont}}^2}{g_{3d}^2}$ as $\frac{\text{Tr}\Phi^2}{g_{3d}^2}$ in the following. The raw data were obtained in separate simulations with $V = N_x^3$. We ensured that the Monte Carlo error of the separate simulations dominates the overall error of $\frac{\text{Tr}\Phi^2}{g_{3d}^2}$, not the uncertainty of y_{crit} . The slightly negative values of $\frac{\text{Tr}\Phi_{\text{symm}}^2}{g_{3d}^2}$ for small x are expected and arise because the positive mass squared at the transition point suppresses IR fluctuations, while the renormalization involves subtracting off large positive counterterms (including the massless, free-theory fluctuations).

2. Transition strength

With the critical values of $\frac{\text{Tr}\Phi^2}{g_{3d}^2}$ in both phases from Table V in hand, we can infer further interesting features of the first-order phase transition. Having several values of $\frac{\text{Tr}\Phi^2}{g_{3d}^2}$ at the same physical x and different lattice spacings $g_{3d}^2 a$, we extrapolate both the difference between phases $\frac{\Delta\text{Tr}\Phi^2}{g_{3d}^2}$ and the symmetric phase value $\frac{\text{Tr}\Phi_{\text{symm}}^2}{g_{3d}^2}$ to the continuum. We provide the former in Fig. 5 and the latter in Fig. 6. The continuum limits, and the linear coefficient in the fit for the case of $\frac{\text{Tr}\Phi_{\text{symm}}^2}{g_{3d}^2}$, are provided in Table VI.

The limiting values of the fits provide us with two interesting pieces of information about the phase transition in this theory. The most interesting is $\frac{\Delta\text{Tr}\Phi^2}{g_{3d}^2}$, which measures the strength of the phase transition. For small x we can predict this strength perturbatively; the limiting behavior is

[28] $\frac{\Delta\text{Tr}\Phi^2}{g_{3d}^2} = 3/(8\pi^2 x^2)$, which we also include in the last frame of Fig. 5. We have provided a cubic fit to guide the eye, but it should not be taken seriously; the strength of the phase transition is a nonperturbative quantity, and there is no reason to expect it to take such a simple form. In fact, we know that $\frac{\Delta\text{Tr}\Phi^2}{g_{3d}^2} \rightarrow 0$ as $x \rightarrow x_{\text{triple}}$, with a nontrivial critical exponent. Note that in the fit for the a dependence of $\frac{\Delta\text{Tr}\Phi^2}{g_{3d}^2}$, we have fitted to a polynomial without a linear term; this is because the known $\mathcal{O}(a)$ corrections are sufficient to eliminate such a linear correction in the *difference* between phases of $\frac{\text{Tr}\Phi^2}{g_{3d}^2}$.

3. Additive operator improvement

On the other hand, the value of either $\frac{\text{Tr}\Phi_{\text{symm}}^2}{g_{3d}^2}$ or $\frac{\text{Tr}\Phi_{\text{brok}}^2}{g_{3d}^2}$, by itself, still contains $\mathcal{O}(a)$ errors, since there is an unknown additive renormalization to the operator $\text{Tr}\Phi^2$ which arises at three loops. Since the correction is additive and both phases were explored at the same y value, these effects cancel in the difference. We took advantage of this cancellation in the last subsection. But now our goal is to use this linear behavior to extract the unknown $\mathcal{O}(a)$ additive corrections to the Φ^2 operator. These arise at three loops in a perturbative lattice-continuum matching calculation, which is prohibitive; so we will again try to extract them from the data.

Because we are working to three loops, we must specify quite carefully how one-loop multiplicative effects will be implemented, since they can multiply one- and two-loop additive effects to give three-loop level contributions, which then differ depending on our exact procedure. Here we will depart slightly from the procedure of Refs. [22,23,35]. We write the continuum expectation value as

$$\frac{\text{Tr}\Phi_{\text{cont}}^2}{g_{3d}^2} = Z_m \left(Z_\Phi \text{Tr}\Phi_{\text{L}}^2 - \frac{\delta\Phi^2}{g_{3d}^2} \right), \quad (\text{B1})$$

where Z_m is the one-loop multiplicative renormalization factor of the $\text{Tr}\Phi^2$ operator, and Z_Φ accounts for our choice of scalar field normalization on the lattice [see Eq. (2.2)]. Examining the three-loop diagrams, we find that certain three-loop effects are absorbed if we define Z_m , *resumming* the Dyson series. That is, in Fig. 7, we take the operator inserted on the one-loop diagrams to be the resummed, rather than the bare, operator, which will sum the Dyson series,

FIG. 7. Diagrams generating Z_m the multiplicative $\text{Tr}\Phi^2$ operator renormalization. Heavy crosses are the renormalized operator (with Z_m factor), while light crosses are the bare operator.

TABLE VII. Covariance matrix of the grand fit of the missing three-loop $\frac{\delta\Phi^2}{g_{3d}^2}$ -contribution.

$\text{cov}(C_i, C_j)$	C_{Φ_a}	C_{Φ_b}	C_{Φ_c}
C_{Φ_a}	21694	-267617	5.3859×10^{-6}
C_{Φ_b}	-267617	3.4914×10^6	-1.432×10^{-4}
C_{Φ_c}	5.3859×10^{-6}	-1.432×10^{-4}	9.0×10^{-4}

leading to an expression for Z_m^{-1} . Slightly rearranging Eqs. (32) and (33) of Ref. [22], we find

$$Z_m^{-1} = 1 + \frac{g_{3d}^2 a}{4\pi} \left(3N\xi + \frac{N\Sigma}{6} - (N^2 + 1)\xi x \right). \quad (\text{B2})$$

Here $\xi = 0.152859324966$ and $\Sigma = 3.17591153562522$ are standard integrals encountered in the one-loop lattice-continuum matching. We are also writing the number of colors $N = 3$ explicitly, to show the detailed dependence on the number of colors. With this definition, the two-loop and partially three-loop result for $\delta\Phi^2$ is

$$\begin{aligned} \frac{\delta\Phi^2}{g_{3d}^2} = & \frac{N^2 - 1}{2g_{3d}^2 a} \left[\frac{\Sigma}{4\pi} - \frac{\xi y g_{3d}^4 a^2}{4\pi} \right. \\ & + \frac{N g_{3d}^2 a}{(4\pi)^2} Z_m^{-1} \left(2 \ln \frac{6}{g_{3d}^2 a} + 2\zeta - 2\delta + \frac{\Sigma^2}{2} \right) \\ & + \frac{g_{3d}^4 a^2}{(4\pi)^3} (2\xi(N^2 + 1)(x^2 - Nx) \ln(g_{3d}^2 a) \\ & \left. + C_{\Phi_a} + C_{\Phi_b} x + C_{\Phi_c} x^2 \right). \quad (\text{B3}) \end{aligned}$$

The unknown coefficients C_{Φ_a} , C_{Φ_b} , and C_{Φ_c} capture the remaining $\mathcal{O}(a)$ corrections from three-loop diagrams which are not iterations of simpler one- and two-loop diagrams. Note that Eq. (B3) contains several terms proportional to $\ln(g_{3d}^2 a)$. These arise from logarithmic divergences in the continuum theory, regulated at our choice of renormalization point $\mu = g_{3d}^2$ but then cut off on the lattice at the scale $1/a$. The term next to $\zeta - \delta$ is the explicit μ^2 dependence of Φ^2/g_{3d}^2 and is therefore expected; the coefficient Z_m^{-1} ensures that it enters Eq. (B1) with precisely the right continuum

normalization. The log terms proportional to ξ in the last line cancel the μ dependence of the mass squared (y) in the mass-dependent $\mathcal{O}(a)$ shift in the first line.

It remains to determine the three coefficients in the last line. In fact, we only need to fit two of these coefficients; one of them, C_{Φ_c} , represents pure-scalar corrections, which can be extracted from Ref. [35]. The reference performs the calculation for an improved hopping term, but repeating the calculation for the nearest-neighbor hopping term we use here,⁴ we find that

$$C_{\Phi_c} = 2(N^2 + 1)C_4, \quad C_4 = 0.5630(4), \quad (\text{B4})$$

which differs from the result in the reference, $C_{4,\text{Ref}} = 0.2817$, because of the different scalar dispersion between the nearest-neighbor hopping term used here and the improved hopping term used there.⁵

After performing these subtractions, we can fit the residual linear a -dependence of $\text{Tr}\Phi_L^2$ for each x value we consider and extract the coefficients C_{Φ_a} , C_{Φ_b} from a grand fit in complete analogy with the m^2 effects we consider in the main text. We find

$$C_{\Phi_a} = (-21 \pm 37), \quad (\text{B5})$$

$$C_{\Phi_b} = (6.7 \pm 4.7) \times 10^2, \quad (\text{B6})$$

again by constrained curve fitting. The grand fit is displayed in the seventh frame of Fig. 6. Unfortunately, it appears that our results fail to constrain these coefficients very much. The full covariance matrix can be found in Table VII. From the covariance matrix, we can also see that the error of C_{Φ_c} is by far the smallest, so the value and error of C_{Φ_c} were not changed by the constrained fit.

⁴The rest of the $\mathcal{O}(a)$ corrections are not known for improved actions, which is why we do not attempt to use an improved action here. Using improved actions really helps only if one can complete the two-loop $\mathcal{O}(a^2)$ matching calculation; this is feasible in a scalar theory, but does not appear practical in a gauge theory as we consider here.

⁵Specifically, in passing from the improved to the unimproved hopping term, Ref. [35] (B38) has $0.30837 \rightarrow 0.2268854$; (B40) has $0.00031757 \rightarrow 0.000490546$, the value of ξ changes from $\xi = -0.08365 \rightarrow +0.1528593$, and (B41) changes from $0.0985(6) \rightarrow 0.1063(4)$.

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